



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:47 PM UTC

PDB ID : 7EH2 / pdb_00007eh2
Title : Thermus thermophilus transcription initiation complex containing a template-strand pyrimidine at position TSS-2 and GpG RNA primer
Authors : Li, L.; Zhang, Y.
Deposited on : 2021-03-27
Resolution : 3.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

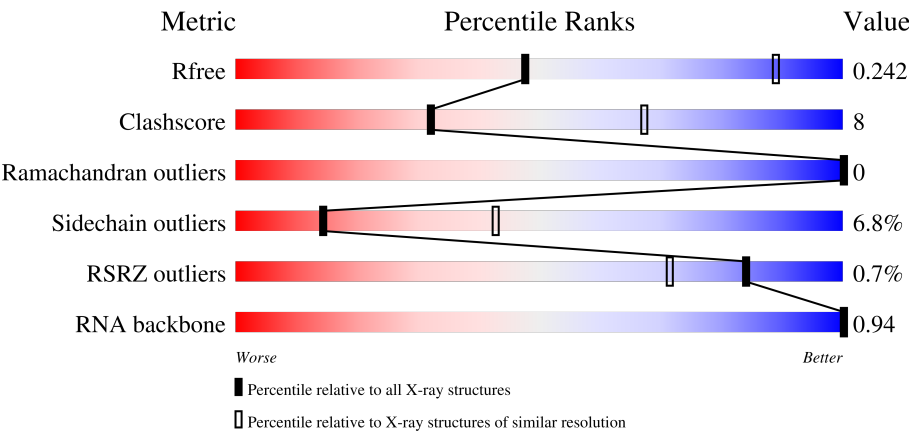
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)
RNA backbone	3983	1083 (3.68-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	50%21%•27%
1	B	315	% 52%17%•30%
1	K	315	54%16%•28%
1	L	315	52%18%•29%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	27	
6	J	27	
7	H	19	
7	Q	19	
8	I	2	
8	R	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 56841 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1777	1136	306	333	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	227	Total	C	N	O	S	0	0	0
			1781	1138	308	333	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8742	5534	1552	1632	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8724	5520	1551	1629	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	0	0
			11680	7405	2051	2189	35			
3	N	1486	Total	C	N	O	S	0	0	0
			11675	7402	2047	2191	35			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2803	1768	509	522	4			
5	P	347	Total	C	N	O	S	0	0	0
			2757	1738	490	525	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
P	-19	MET	-	expression tag	UNP Q5SKW1
P	-18	GLY	-	expression tag	UNP Q5SKW1
P	-17	SER	-	expression tag	UNP Q5SKW1
P	-16	SER	-	expression tag	UNP Q5SKW1
P	-15	HIS	-	expression tag	UNP Q5SKW1
P	-14	HIS	-	expression tag	UNP Q5SKW1
P	-13	HIS	-	expression tag	UNP Q5SKW1
P	-12	HIS	-	expression tag	UNP Q5SKW1
P	-11	HIS	-	expression tag	UNP Q5SKW1
P	-10	HIS	-	expression tag	UNP Q5SKW1
P	-9	SER	-	expression tag	UNP Q5SKW1
P	-8	SER	-	expression tag	UNP Q5SKW1
P	-7	GLY	-	expression tag	UNP Q5SKW1
P	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	expression tag	UNP Q5SKW1
P	-4	PRO	-	expression tag	UNP Q5SKW1
P	-3	ARG	-	expression tag	UNP Q5SKW1
P	-2	GLY	-	expression tag	UNP Q5SKW1
P	-1	SER	-	expression tag	UNP Q5SKW1
P	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			
6	J	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

- Molecule 7 is a DNA chain called DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*CP*CP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			
7	Q	17	Total	C	N	O	P	0	0	0
			345	165	63	101	16			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			
8	R	2	Total	C	N	O	P	0	0	0
			43	20	10	12	1			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total Mg 1 1	0	0
10	L	1	Total Mg 1 1	0	0
10	N	1	Total Mg 1 1	0	0

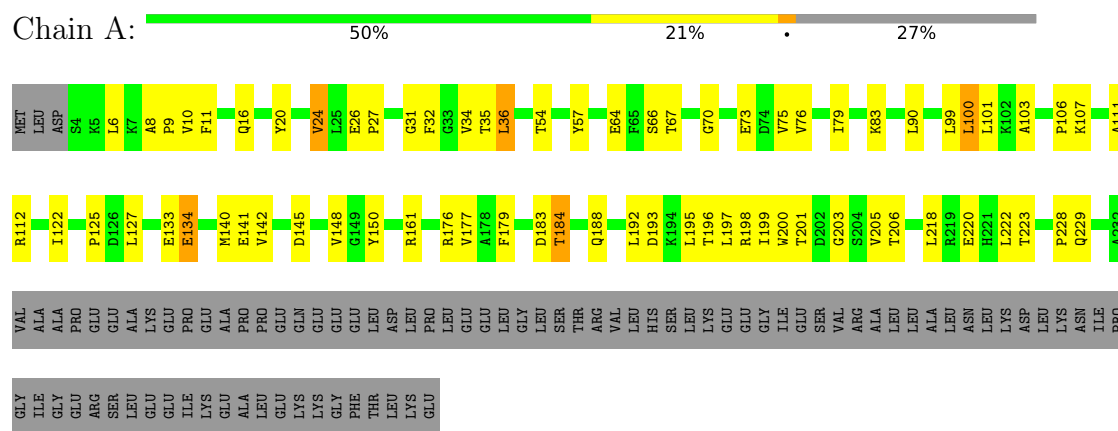
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	4	Total O 4 4	0	0
11	B	4	Total O 4 4	0	0
11	C	5	Total O 5 5	0	0
11	D	10	Total O 10 10	0	0
11	E	2	Total O 2 2	0	0
11	F	1	Total O 1 1	0	0
11	K	2	Total O 2 2	0	0
11	L	1	Total O 1 1	0	0
11	M	1	Total O 1 1	0	0
11	N	9	Total O 9 9	0	0
11	O	2	Total O 2 2	0	0
11	G	1	Total O 1 1	0	0

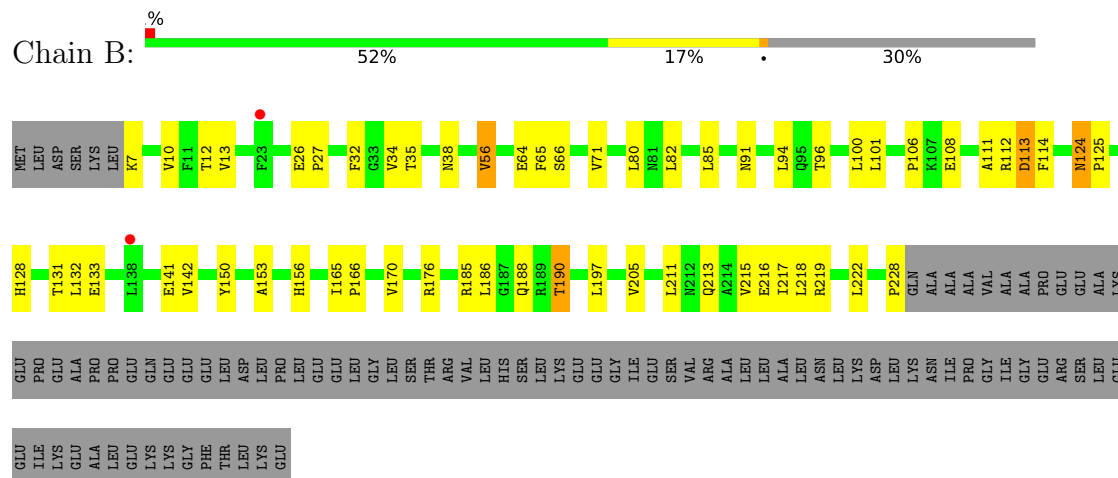
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

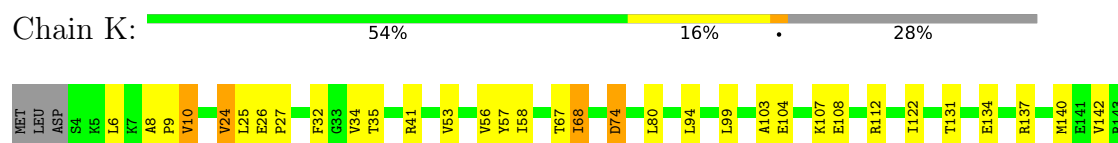
• Molecule 1: DNA-directed RNA polymerase subunit alpha

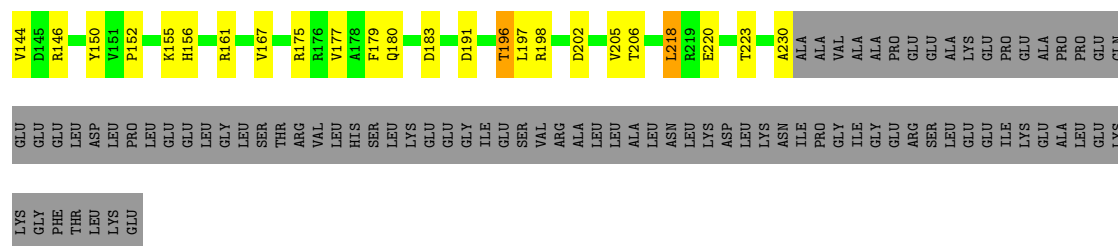


• Molecule 1: DNA-directed RNA polymerase subunit alpha



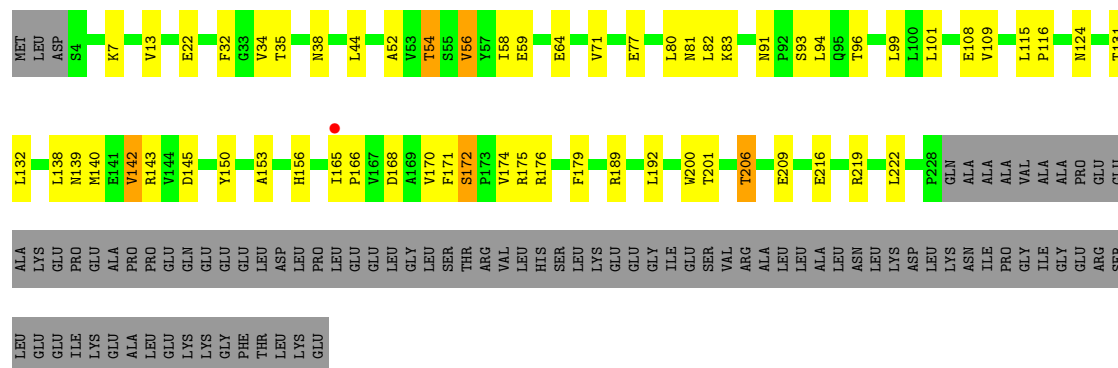
• Molecule 1: DNA-directed RNA polymerase subunit alpha





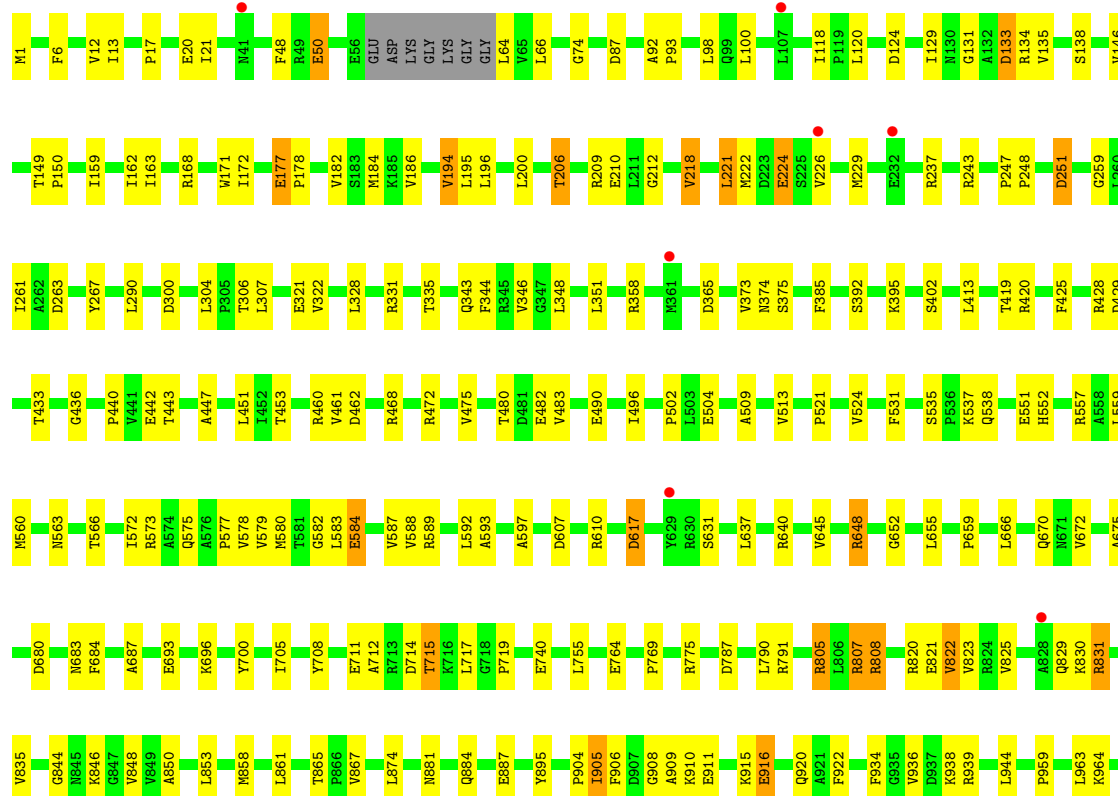
• Molecule 1: DNA-directed RNA polymerase subunit alpha

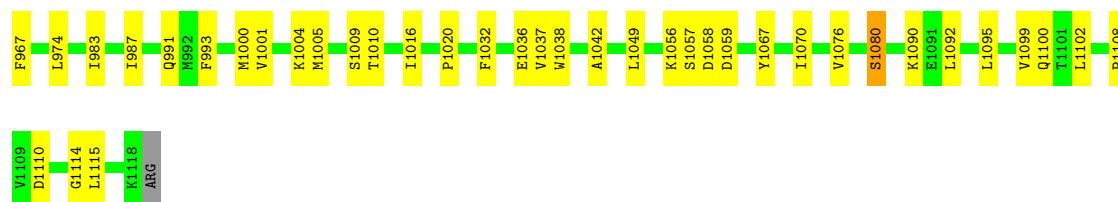
Chain L: 52% 18% 29%



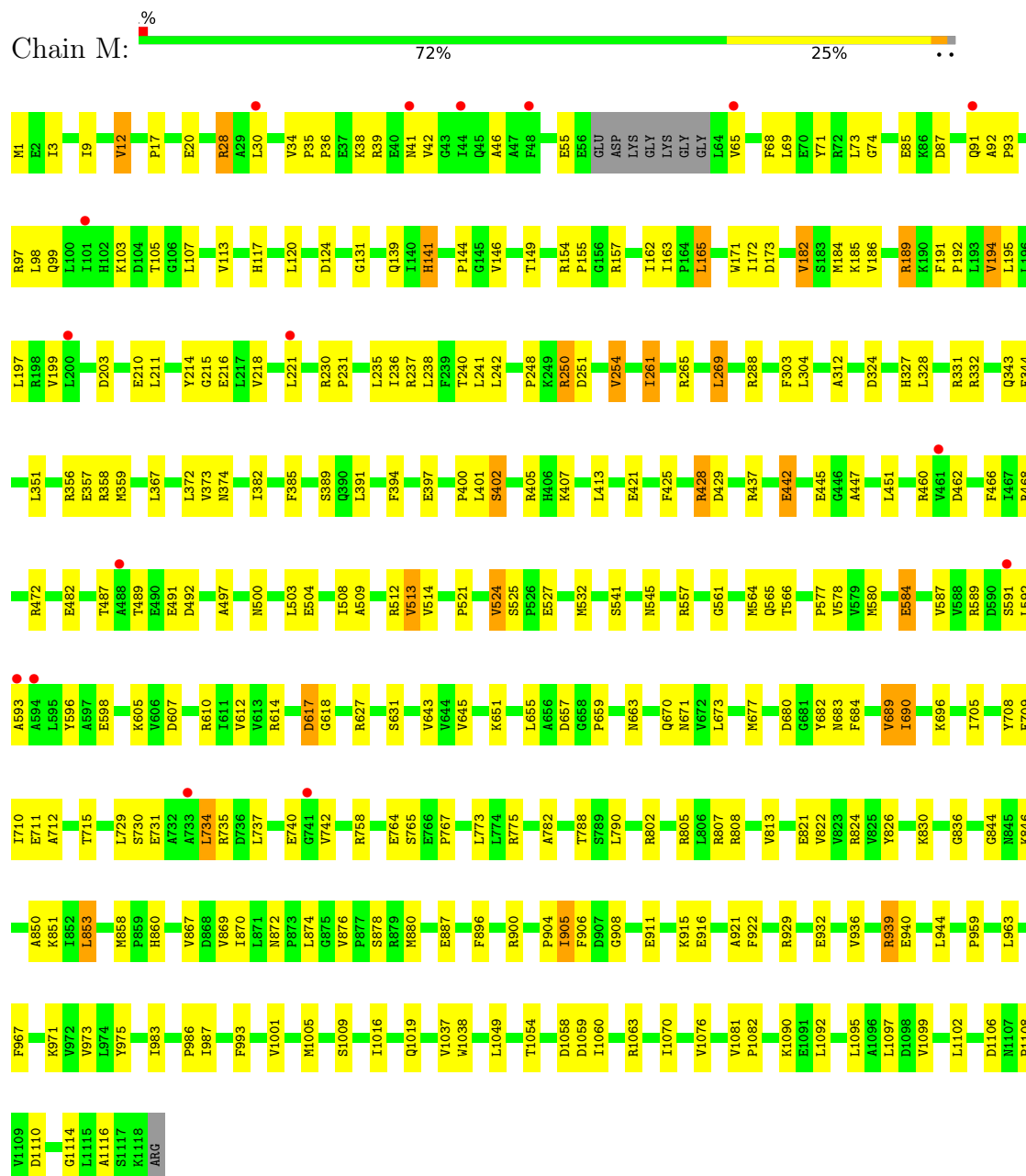
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 76% 22%

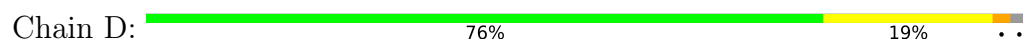


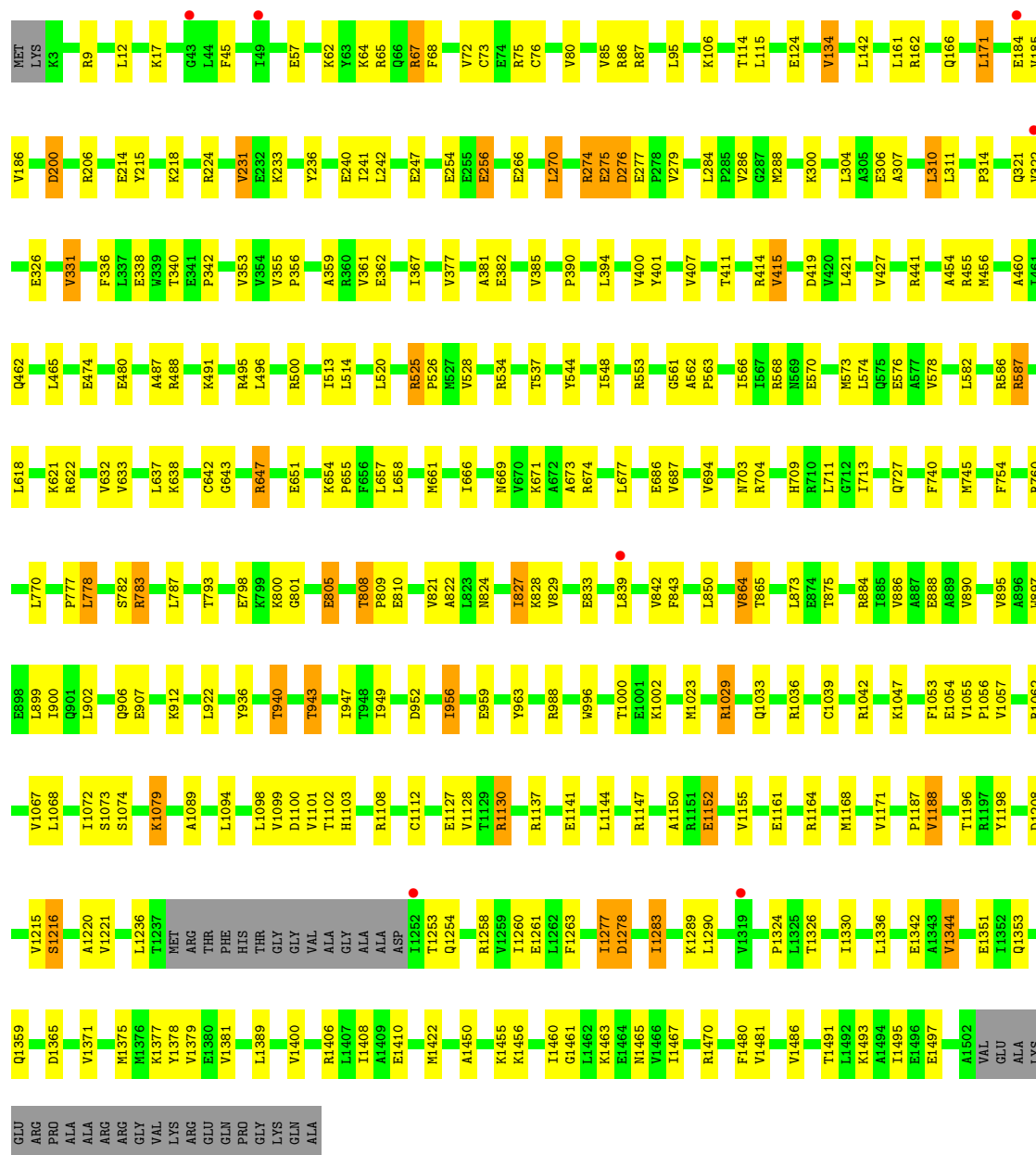


• Molecule 2: DNA-directed RNA polymerase subunit beta

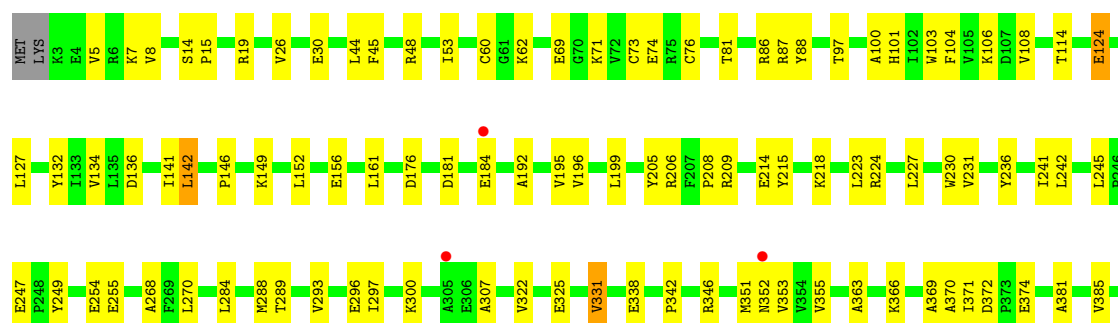
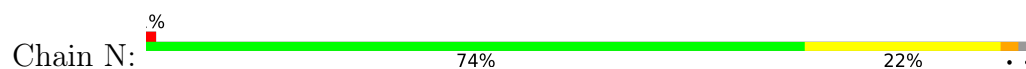


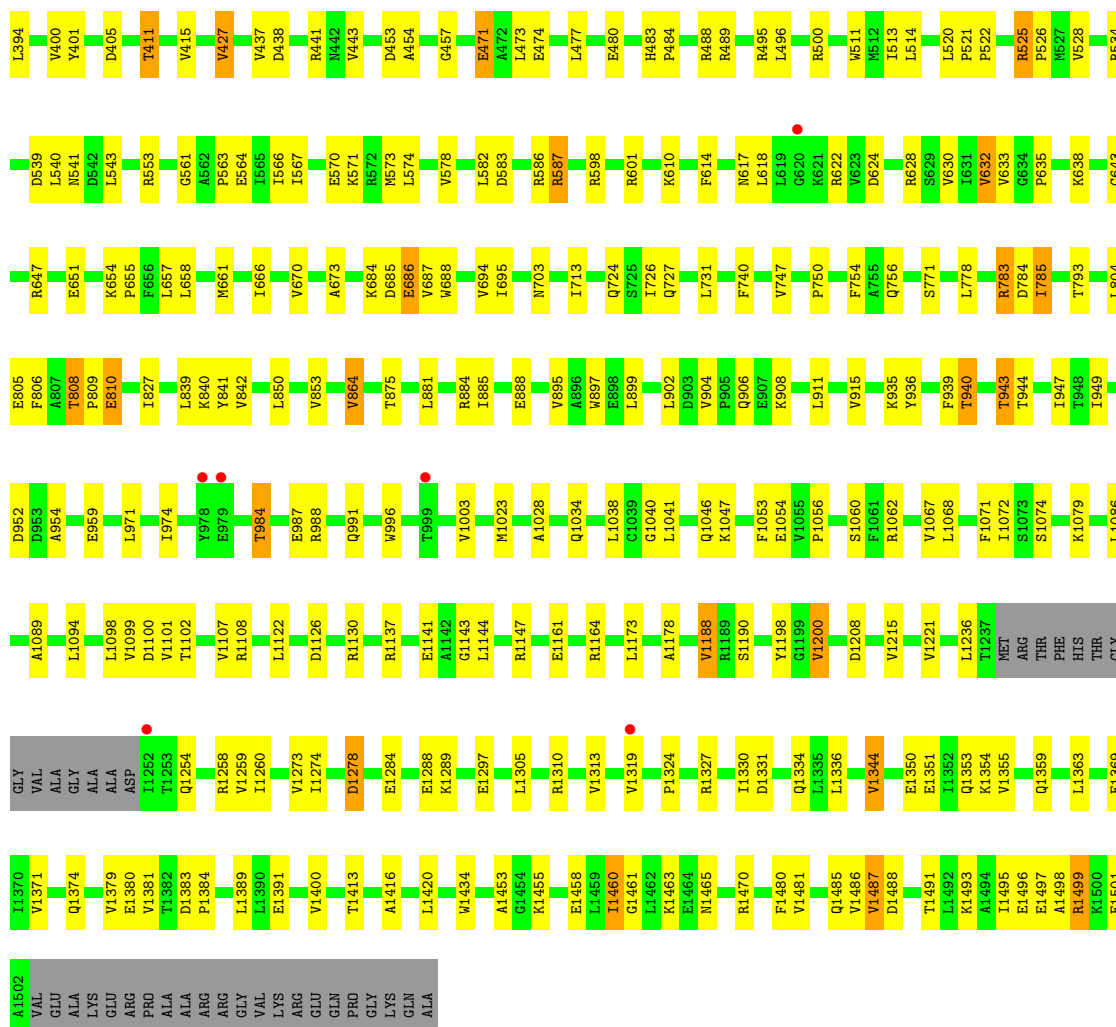
• Molecule 3: DNA-directed RNA polymerase subunit beta'





• Molecule 3: DNA-directed RNA polymerase subunit beta'





- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 72% 22% 5%



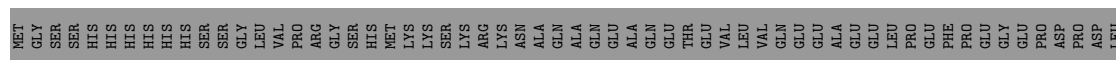
- Molecule 4: DNA-directed RNA polymerase subunit omega

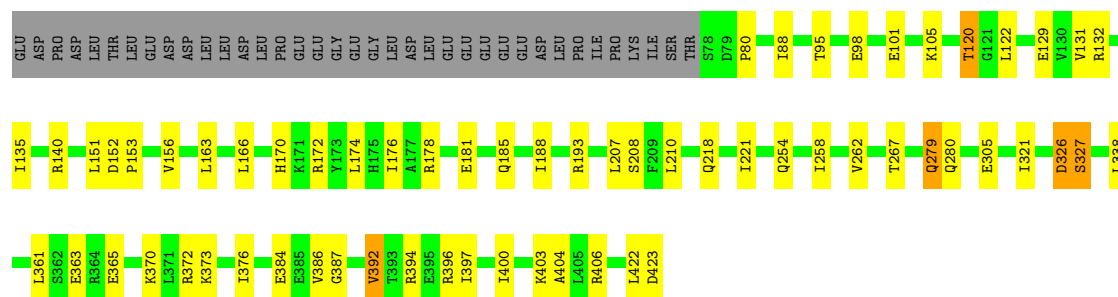
Chain O: 71% 23% 5%



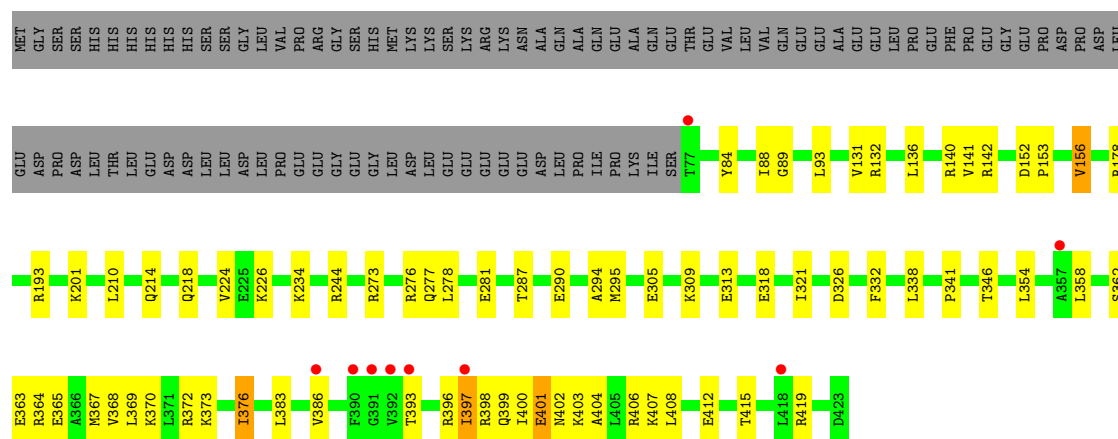
- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 64% 13% 22%





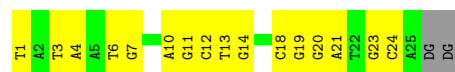
• Molecule 5: RNA polymerase sigma factor SigA



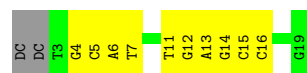
• Molecule 6: DNA (27-MER)



• Molecule 6: DNA (27-MER)

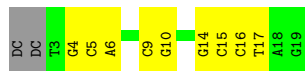


• Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*AP*G)-3')

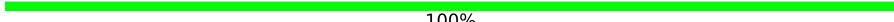


- Molecule 7: DNA (5'-D(*CP*C*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*CP*CP*TP*AP*G)-3')

Chain Q:  42% 47% 11%



- Molecule 8: RNA (5'-R(*GP*G)-3')

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: RNA (5'-R(*GP*G)-3')

Chain R:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	184.85Å 104.20Å 296.65Å 90.00° 98.42° 90.00°	Depositor
Resolution (Å)	97.82 – 3.34 97.82 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (97.82-3.34) 99.6 (97.82-3.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.201 , 0.247 (Not available) , 0.242	Depositor DCC
R_{free} test set	8256 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56841	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8581e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/1809	0.36	0/2464
1	B	0.12	0/1782	0.35	0/2424
1	K	0.13	0/1813	0.39	0/2466
1	L	0.14	0/1805	0.39	0/2454
2	C	0.13	0/8909	0.36	0/12054
2	M	0.14	0/8890	0.37	0/12030
3	D	0.14	0/11885	0.36	0/16081
3	N	0.13	0/11880	0.35	0/16074
4	E	0.12	0/775	0.31	0/1045
4	O	0.13	0/775	0.33	0/1045
5	F	0.14	0/2848	0.35	0/3832
5	P	0.14	0/2800	0.33	0/3777
6	G	0.19	0/580	0.42	0/895
6	J	0.20	0/580	0.43	0/895
7	H	0.20	0/386	0.39	0/594
7	Q	0.20	0/386	0.38	0/594
8	I	0.12	0/48	0.28	0/74
8	R	0.14	0/48	0.32	0/74
All	All	0.14	0/57999	0.36	0/78872

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	274	ARG	Peptide
3	D	276	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1812	43	0
1	B	1750	0	1797	32	0
1	K	1781	0	1828	32	0
1	L	1773	0	1826	35	0
2	C	8742	0	8826	143	0
2	M	8724	0	8795	174	0
3	D	11680	0	11864	192	0
3	N	11675	0	11851	211	0
4	E	761	0	778	14	0
4	O	761	0	778	14	0
5	F	2803	0	2878	38	0
5	P	2757	0	2780	47	0
6	G	516	0	283	10	0
6	J	516	0	283	15	0
7	H	345	0	193	9	0
7	Q	345	0	193	10	0
8	I	43	0	23	0	0
8	R	43	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	1	0	0	0	0
10	L	1	0	0	0	0
10	N	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0
11	C	5	0	0	0	0
11	D	10	0	0	0	0
11	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	1	0	0	0	0
11	G	1	0	0	0	0
11	K	2	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	9	0	0	3	0
11	O	2	0	0	0	0
All	All	56841	0	56811	910	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (910) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.58	0.84
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.62	0.81
2:M:683:ASN:HB3	2:M:872:ASN:HB2	1.61	0.81
5:P:408:LEU:O	5:P:412:GLU:HB2	1.83	0.77
3:N:60:CYS:SG	11:N:1702:HOH:O	2.43	0.76
3:D:1112:CYS:HB3	3:D:1196:THR:HG23	1.67	0.75
3:N:142:LEU:HB2	3:N:161:LEU:HD21	1.68	0.74
2:M:154:ARG:HE	2:M:157:ARG:HG3	1.50	0.74
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.70	0.73
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.71	0.72
3:N:73:CYS:SG	11:N:1702:HOH:O	2.47	0.72
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.23	0.71
2:M:689:VAL:HG13	2:M:851:LYS:HB3	1.72	0.71
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.72	0.71
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.73	0.71
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.73	0.71
1:B:32:PHE:HA	1:B:35:THR:HB	1.72	0.70
3:N:1324:PRO:HG3	3:N:1330:ILE:HD11	1.72	0.70
2:C:1005:MET:HE1	3:D:647:ARG:HB2	1.74	0.70
2:M:557:ARG:HG3	2:M:844:GLY:HA3	1.74	0.70
3:N:520:LEU:HD23	3:N:525:ARG:HG2	1.74	0.69
2:M:428:ARG:NH2	2:M:447:ALA:O	2.24	0.69
3:D:162:ARG:O	3:D:414:ARG:NH1	2.26	0.69
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.75	0.69
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.75	0.69
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:256:GLU:O	3:D:274:ARG:NH2	2.25	0.68
2:C:428:ARG:NH2	2:C:447:ALA:O	2.27	0.68
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.76	0.68
5:P:136:LEU:HD13	5:P:140:ARG:HG2	1.76	0.68
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.76	0.68
3:N:1498:ALA:HB1	4:O:84:ARG:HH21	1.58	0.68
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.26	0.68
2:M:172:ILE:HG13	2:M:186:VAL:HG22	1.76	0.67
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.77	0.67
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.76	0.67
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.77	0.67
5:P:354:LEU:O	5:P:358:LEU:HB2	1.94	0.67
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.76	0.67
2:M:905:ILE:HG23	2:M:906:PHE:HD1	1.60	0.67
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.76	0.66
3:D:809:PRO:HB3	3:D:839:LEU:HD13	1.76	0.66
2:M:189:ARG:HH12	2:M:242:LEU:HA	1.58	0.66
2:M:874:LEU:HD13	3:N:783:ARG:HB2	1.78	0.66
3:N:288:MET:HE2	3:N:307:ALA:HB2	1.78	0.66
6:J:3:DT:H2'	6:J:4:DA:C8	2.30	0.66
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.76	0.66
1:L:32:PHE:HA	1:L:35:THR:HB	1.76	0.66
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.29	0.66
3:D:1033:GLN:OE1	3:D:1036:ARG:NH1	2.29	0.66
3:N:750:PRO:O	3:N:756:GLN:NE2	2.30	0.65
2:M:680:ASP:H	3:N:943:THR:CG2	2.08	0.65
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.30	0.65
3:D:798:GLU:HG3	3:D:824:ASN:HB2	1.78	0.65
3:N:984:THR:HG22	3:N:987:GLU:HG3	1.77	0.65
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.78	0.65
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.28	0.65
2:M:144:PRO:HG2	2:M:165:LEU:HD23	1.78	0.64
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.80	0.64
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.79	0.64
1:B:112:ARG:HG3	1:B:125:PRO:HB2	1.79	0.64
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.79	0.64
2:M:876:VAL:HB	3:N:949:ILE:HD12	1.80	0.64
3:D:326:GLU:HG2	3:D:331:VAL:HG13	1.80	0.63
5:P:273:ARG:HG2	5:P:276:ARG:HH12	1.64	0.63
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.81	0.63
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:905:ILE:HG23	2:C:906:PHE:HD2	1.64	0.62
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.31	0.62
1:K:9:PRO:HB3	1:K:27:PRO:HD2	1.82	0.62
1:K:104:GLU:OE2	1:K:137:ARG:NH1	2.33	0.62
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.79	0.62
2:C:617:ASP:OD1	2:C:617:ASP:N	2.32	0.62
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.33	0.62
2:C:911:GLU:O	2:C:915:LYS:HG2	2.00	0.62
5:P:370:LYS:HB3	5:P:376:ILE:HD13	1.81	0.62
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.82	0.62
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.82	0.62
1:L:206:THR:HG22	1:L:209:GLU:H	1.63	0.62
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.64	0.62
2:M:684:PHE:HB3	3:N:633:VAL:HG21	1.81	0.61
2:M:397:GLU:HG3	2:M:631:SER:HB2	1.82	0.61
3:D:520:LEU:O	3:D:525:ARG:NH1	2.32	0.61
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.83	0.61
1:K:32:PHE:HA	1:K:35:THR:HB	1.82	0.61
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.83	0.61
3:N:270:LEU:HG	3:N:284:LEU:HD11	1.81	0.61
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.83	0.61
7:H:15:DC:H2'	7:H:16:DC:C6	2.36	0.61
6:J:23:DG:H2''	6:J:24:DC:H5''	1.83	0.61
3:N:1101:VAL:HG13	3:N:1102:THR:HG23	1.83	0.61
1:B:153:ALA:HA	1:B:156:HIS:CD2	2.36	0.61
3:N:771:SER:HB2	3:N:778:LEU:HG	1.82	0.60
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.82	0.60
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.84	0.60
2:C:874:LEU:HD13	3:D:783:ARG:HB2	1.82	0.60
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.84	0.60
3:N:949:ILE:HD11	3:N:1023:MET:HE1	1.82	0.60
1:A:32:PHE:HA	1:A:35:THR:HB	1.84	0.60
2:M:758:ARG:HH21	2:M:788:THR:HB	1.66	0.60
3:N:351:MET:HE3	3:N:370:ALA:HB2	1.82	0.60
3:N:534:ARG:NH2	5:P:313:GLU:O	2.35	0.60
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.84	0.60
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.84	0.59
7:H:15:DC:H2'	7:H:16:DC:H6	1.67	0.59
1:A:9:PRO:HB3	1:A:27:PRO:HD2	1.85	0.59
4:E:39:VAL:O	4:E:72:ARG:NH1	2.31	0.59
3:N:657:LEU:HG	3:N:661:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:GLU:OE2	2:C:168:ARG:NH1	2.35	0.59
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.59
3:D:288:MET:HA	3:D:306:GLU:O	2.02	0.59
2:M:182:VAL:HG13	2:M:221:LEU:HD13	1.83	0.59
5:P:403:LYS:HA	5:P:406:ARG:HG2	1.84	0.59
3:D:1152:GLU:HG2	3:D:1161:GLU:HA	1.84	0.59
6:J:12:DC:H4'	6:J:13:DT:H5'	1.84	0.59
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.85	0.59
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.34	0.59
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.84	0.59
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.83	0.59
3:N:480:GLU:OE2	3:N:488:ARG:NH2	2.35	0.59
3:N:793:THR:HG21	3:N:906:GLN:HG2	1.85	0.59
5:P:131:VAL:HG13	5:P:178:ARG:HD3	1.83	0.59
3:N:785:ILE:HD12	3:N:935:LYS:HA	1.85	0.59
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.85	0.59
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.85	0.59
2:C:916:GLU:OE1	2:C:920:GLN:NE2	2.32	0.59
3:N:1003:VAL:HG21	3:N:1041:LEU:HG	1.85	0.59
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.85	0.58
5:P:226:LYS:HD3	6:J:1:DT:H73	1.85	0.58
5:P:362:SER:HB3	5:P:365:GLU:HG3	1.85	0.58
7:Q:14:DG:H2'	7:Q:15:DC:H6	1.67	0.58
2:M:87:ASP:HA	2:M:131:GLY:HA3	1.84	0.58
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.85	0.58
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.35	0.58
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.85	0.58
3:N:400:VAL:HG13	3:N:443:VAL:HG21	1.84	0.58
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.85	0.58
2:C:769:PRO:HG3	3:D:65:ARG:HH11	1.67	0.58
2:C:1067:TYR:OH	3:D:674:ARG:NH1	2.37	0.58
2:M:55:GLU:HA	2:M:65:VAL:HG22	1.86	0.58
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.86	0.58
2:M:1054:THR:HG22	2:M:1082:PRO:HG3	1.85	0.58
5:F:386:VAL:HB	5:F:397:ILE:HG21	1.85	0.58
2:M:971:LYS:HB3	2:M:986:PRO:HB2	1.86	0.58
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.68	0.57
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.86	0.57
2:M:614:ARG:NH2	2:M:618:GLY:O	2.37	0.57
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.37	0.57
3:N:601:ARG:HD3	5:P:318:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.86	0.57
4:E:50:THR:OG1	4:E:51:LEU:N	2.37	0.57
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.86	0.57
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.87	0.57
2:C:420:ARG:HD3	2:C:447:ALA:HB1	1.87	0.56
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.86	0.56
2:M:513:VAL:HG22	2:M:524:VAL:HG12	1.86	0.56
4:E:57:ASP:O	4:E:63:TRP:NE1	2.35	0.56
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.88	0.56
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.87	0.56
5:F:326:ASP:OD1	5:F:326:ASP:N	2.34	0.56
1:K:94:LEU:O	1:K:146:ARG:NH1	2.36	0.56
2:M:593:ALA:HB1	2:M:659:PRO:HD2	1.87	0.56
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.88	0.56
1:L:175:ARG:N	1:L:200:TRP:O	2.32	0.56
3:D:288:MET:HE3	3:D:307:ALA:HB2	1.87	0.56
5:P:140:ARG:HG3	5:P:142:ARG:HH22	1.71	0.56
6:G:12:DC:H4'	6:G:13:DT:H5'	1.88	0.56
1:B:113:ASP:OD1	1:B:113:ASP:N	2.39	0.56
1:L:101:LEU:HD21	1:L:109:VAL:HG11	1.88	0.55
1:L:153:ALA:HB1	1:L:166:PRO:HB2	1.88	0.55
2:M:195:LEU:HD23	2:M:238:LEU:HD13	1.86	0.55
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.87	0.55
1:L:153:ALA:HA	1:L:156:HIS:CD2	2.42	0.55
5:P:396:ARG:HH21	5:P:400:ILE:HD12	1.69	0.55
3:D:805:GLU:OE2	3:D:828:LYS:NZ	2.31	0.55
1:L:91:ASN:HB3	1:L:94:LEU:HB2	1.87	0.55
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	1.89	0.55
3:N:1137:ARG:O	3:N:1141:GLU:HG3	2.07	0.55
6:J:10:DA:H2''	6:J:11:DG:C8	2.42	0.55
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.89	0.55
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.39	0.55
1:K:74:ASP:HB3	2:M:627:ARG:HH12	1.72	0.55
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.89	0.55
3:N:574:LEU:O	3:N:578:VAL:HG23	2.06	0.55
6:G:23:DG:H2''	6:G:24:DC:H5''	1.88	0.55
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.88	0.55
3:D:520:LEU:HD23	3:D:525:ARG:HG2	1.89	0.54
1:K:74:ASP:OD1	1:K:74:ASP:N	2.37	0.54
3:N:231:VAL:O	3:N:236:TYR:OH	2.20	0.54
2:M:617:ASP:OD1	2:M:617:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:680:ASP:H	3:N:943:THR:HG21	1.72	0.54
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.90	0.54
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.89	0.54
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.08	0.54
2:M:680:ASP:H	3:N:943:THR:HG22	1.71	0.54
7:Q:14:DG:H2'	7:Q:15:DC:C6	2.41	0.54
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.90	0.54
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.38	0.54
2:C:1059:ASP:OD2	2:C:1080:SER:N	2.39	0.54
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.40	0.54
4:O:48:MET:HE2	4:O:50:THR:HG22	1.90	0.54
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.43	0.54
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.40	0.54
2:M:904:PRO:HD2	2:M:908:GLY:HA2	1.88	0.54
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.89	0.54
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.90	0.54
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.89	0.54
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.90	0.54
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.90	0.54
3:N:632:VAL:N	3:N:726:ILE:O	2.40	0.54
6:J:18:DC:H2''	6:J:19:DG:C8	2.43	0.54
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.88	0.54
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.42	0.54
3:N:633:VAL:HG13	3:N:635:PRO:HD3	1.88	0.54
3:D:275:GLU:HG2	3:D:276:ASP:N	2.23	0.54
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.90	0.54
3:D:782:SER:OG	3:D:783:ARG:N	2.41	0.54
2:M:911:GLU:O	2:M:915:LYS:HG2	2.08	0.54
7:Q:15:DC:H2'	7:Q:16:DC:H6	1.73	0.53
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.90	0.53
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.90	0.53
1:L:52:ALA:HB2	1:L:171:PHE:HA	1.89	0.53
1:L:99:LEU:HB2	1:L:142:VAL:HG22	1.90	0.53
3:N:1100:ASP:OD2	3:N:1463:LYS:NZ	2.34	0.53
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.91	0.53
1:A:70:GLY:N	2:C:607:ASP:OD1	2.42	0.53
2:C:850:ALA:HB1	3:D:633:VAL:HG12	1.90	0.53
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.90	0.53
3:D:233:LYS:NZ	3:D:240:GLU:OE2	2.28	0.53
3:N:809:PRO:HB3	3:N:839:LEU:HD13	1.91	0.53
5:P:193:ARG:HB2	6:J:6:DT:H1'	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.91	0.53
2:C:133:ASP:HB3	2:C:395:LYS:HE3	1.90	0.53
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.91	0.53
2:C:331:ARG:NH2	6:G:14:DG:O6	2.42	0.53
3:D:562:ALA:O	5:F:140:ARG:NH1	2.28	0.53
3:D:1100:ASP:OD2	3:D:1463:LYS:NZ	2.38	0.53
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.42	0.53
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.89	0.53
2:C:587:VAL:HG11	2:C:666:LEU:HD22	1.91	0.53
2:M:331:ARG:NH2	6:J:14:DG:O6	2.41	0.53
3:N:808:THR:HB	3:N:810:GLU:HG2	1.91	0.53
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.24	0.53
5:P:365:GLU:HA	5:P:368:VAL:HG22	1.91	0.53
3:D:671:LYS:NZ	5:F:423:ASP:OD1	2.40	0.52
2:M:69:LEU:HD12	2:M:97:ARG:HG2	1.91	0.52
3:N:134:VAL:HG12	3:N:454:ALA:HB2	1.91	0.52
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.91	0.52
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.91	0.52
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.92	0.52
1:B:124:ASN:OD1	1:B:124:ASN:N	2.41	0.52
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.90	0.52
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.72	0.52
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.91	0.52
2:C:1009:SER:HB3	3:D:651:GLU:O	2.08	0.52
3:D:890:VAL:HB	3:D:922:LEU:HD22	1.92	0.52
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.42	0.52
2:M:171:TRP:CH2	6:J:14:DG:H5'	2.45	0.52
3:D:633:VAL:HA	3:D:740:PHE:CZ	2.45	0.52
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.25	0.52
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.38	0.52
3:D:657:LEU:HG	3:D:661:MET:HE2	1.91	0.52
5:P:326:ASP:OD1	5:P:326:ASP:N	2.39	0.52
2:M:351:LEU:HD21	2:M:373:VAL:HG13	1.92	0.52
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.91	0.52
2:M:1038:TRP:CE2	3:N:1099:VAL:HG11	2.45	0.52
2:M:1095:LEU:HD23	3:N:582:LEU:HD22	1.91	0.52
3:N:45:PHE:O	3:N:86:ARG:NH2	2.42	0.52
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.92	0.52
2:M:836:GLY:HA3	2:M:1001:VAL:HG21	1.90	0.52
6:G:3:DT:H2''	6:G:4:DA:C8	2.45	0.52
6:J:20:DG:H2''	6:J:21:DA:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.90	0.51
1:K:26:GLU:HB3	1:K:27:PRO:HD3	1.91	0.51
7:H:5:DC:H2'	7:H:6:DA:C8	2.45	0.51
3:N:401:TYR:HB3	3:N:427:VAL:HG21	1.93	0.51
3:N:1485:GLN:O	4:O:75:PHE:HA	2.11	0.51
1:K:10:VAL:HG22	1:K:26:GLU:HB3	1.92	0.51
2:M:269:LEU:O	2:M:288:ARG:HD2	2.10	0.51
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.10	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.93	0.51
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.91	0.51
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.45	0.51
6:G:24:DC:H2'	6:G:25:DA:C8	2.45	0.51
1:L:143:ARG:NE	1:L:145:ASP:OD1	2.44	0.51
4:O:66:LYS:O	4:O:70:THR:HG23	2.10	0.51
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.51
5:P:278:LEU:HD11	5:P:294:ALA:HB3	1.92	0.51
2:M:327:HIS:NE2	2:M:492:ASP:OD2	2.36	0.51
5:P:152:ASP:OD1	5:P:152:ASP:N	2.42	0.51
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.93	0.51
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.92	0.51
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.93	0.51
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.91	0.51
3:N:806:PHE:CD1	3:N:827:ILE:HD11	2.46	0.51
3:N:911:LEU:O	3:N:915:VAL:HG23	2.11	0.51
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.92	0.51
3:N:897:TRP:CH2	3:N:902:LEU:HD22	2.46	0.51
7:Q:15:DC:H2'	7:Q:16:DC:C6	2.46	0.51
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.91	0.50
2:M:673:LEU:HD23	2:M:867:VAL:HA	1.93	0.50
6:J:18:DC:H2''	6:J:19:DG:H8	1.75	0.50
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.44	0.50
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.47	0.50
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.77	0.50
1:K:99:LEU:HD21	1:K:122:ILE:HD11	1.93	0.50
3:N:489:ARG:NH1	3:N:1391:GLU:OE2	2.44	0.50
6:J:11:DG:H2'	6:J:12:DC:C4	2.45	0.50
3:D:793:THR:HG21	3:D:906:GLN:HG2	1.94	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.35	0.50
1:A:177:VAL:HG22	1:A:199:ILE:HG12	1.93	0.50
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.92	0.50
2:M:184:MET:HG2	2:M:186:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:45:PHE:CD2	3:N:522:PRO:HB3	2.47	0.50
3:N:1381:VAL:HG21	3:N:1389:LEU:HD23	1.94	0.50
3:D:821:VAL:HG11	3:D:827:ILE:HD11	1.94	0.50
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.93	0.50
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.11	0.50
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.93	0.50
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.12	0.50
3:N:411:THR:HG23	5:P:178:ARG:HB2	1.92	0.50
4:O:37:ASN:HD22	4:O:89:MET:HE1	1.76	0.50
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.93	0.50
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.93	0.50
3:D:828:LYS:HG2	3:D:829:VAL:O	2.12	0.50
3:D:1168:MET:HE3	3:D:1171:VAL:HB	1.94	0.50
3:N:583:ASP:CG	3:N:586:ARG:HG2	2.37	0.50
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.94	0.50
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.77	0.49
3:N:647:ARG:HH11	3:N:724:GLN:HG3	1.76	0.49
5:P:89:GLY:HA3	6:J:7:DG:C6	2.47	0.49
3:N:974:ILE:HD13	3:N:991:GLN:HB3	1.94	0.49
1:A:103:ALA:HB1	1:A:107:LYS:HD3	1.94	0.49
2:C:243:ARG:NH2	6:G:9:DG:O6	2.40	0.49
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.94	0.49
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.93	0.49
1:K:56:VAL:HG23	1:K:167:VAL:HG21	1.93	0.49
2:M:385:PHE:O	2:M:389:SER:HB3	2.12	0.49
3:N:71:LYS:NZ	3:N:74:GLU:OE2	2.36	0.49
3:N:1094:LEU:HD22	3:N:1260:ILE:HG12	1.94	0.49
6:J:10:DA:H2''	6:J:11:DG:H8	1.76	0.49
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.94	0.49
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.46	0.49
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.95	0.49
3:D:936:TYR:O	3:D:940:THR:OG1	2.30	0.49
3:N:438:ASP:OD2	3:N:441:ARG:NH2	2.45	0.49
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.12	0.49
2:C:711:GLU:HG2	2:C:822:VAL:HG23	1.94	0.49
2:M:1063:ARG:HG3	5:P:341:PRO:HG3	1.95	0.49
6:G:18:DC:H2''	6:G:19:DG:C8	2.48	0.49
1:L:216:GLU:OE1	1:L:219:ARG:NH2	2.43	0.49
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.93	0.49
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.95	0.49
3:N:936:TYR:O	3:N:940:THR:OG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.95	0.49
3:D:760:ARG:HH22	4:E:62:THR:HG1	1.59	0.49
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	1.94	0.49
1:K:152:PRO:HD2	1:K:155:LYS:HB2	1.94	0.49
2:M:124:ASP:OD2	2:M:407:LYS:NZ	2.39	0.49
3:N:206:ARG:HD3	3:N:394:LEU:HB2	1.94	0.49
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.95	0.49
2:C:146:VAL:HG11	2:C:306:THR:HG22	1.95	0.48
3:D:1089:ALA:HA	7:H:14:DG:C8	2.47	0.48
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.13	0.48
2:M:690:ILE:HG22	2:M:869:VAL:HG22	1.94	0.48
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.95	0.48
5:P:84:TYR:O	5:P:88:ILE:HG12	2.13	0.48
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.94	0.48
2:C:537:LYS:HD3	2:C:583:LEU:HD11	1.94	0.48
5:F:370:LYS:HB3	5:F:376:ILE:HG13	1.94	0.48
1:L:80:LEU:HD21	3:N:842:VAL:HG12	1.96	0.48
2:M:425:PHE:HE1	3:N:1086:LEU:HD12	1.78	0.48
2:M:497:ALA:HB3	2:M:532:MET:HG3	1.93	0.48
3:N:954:ALA:HB3	3:N:1062:ARG:HD2	1.95	0.48
3:N:1350:GLU:O	3:N:1354:LYS:HG3	2.13	0.48
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.46	0.48
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.13	0.48
2:C:755:LEU:HD22	2:C:825:VAL:HG11	1.95	0.48
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.94	0.48
4:E:49:GLN:NE2	4:E:50:THR:O	2.46	0.48
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.14	0.48
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.95	0.48
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.33	0.48
3:D:544:TYR:O	3:D:548:ILE:HG12	2.13	0.48
2:M:91:GLN:HB2	2:M:117:HIS:HB3	1.95	0.48
3:N:939:PHE:O	3:N:943:THR:HG23	2.14	0.48
3:D:654:LYS:O	3:D:658:LEU:HG	2.14	0.48
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.96	0.48
3:N:245:LEU:HD13	3:N:249:TYR:HB3	1.96	0.48
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.96	0.48
3:N:703:ASN:HB2	3:N:713:ILE:HG12	1.96	0.48
5:P:358:LEU:HD21	5:P:370:LYS:HG3	1.96	0.48
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.96	0.48
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.96	0.48
2:C:218:VAL:O	2:C:222:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.49	0.48
5:F:387:GLY:HA2	5:F:397:ILE:HG13	1.95	0.48
2:M:805:ARG:HE	2:M:807:ARG:HD3	1.79	0.48
2:M:1009:SER:HB3	3:N:651:GLU:O	2.14	0.48
3:N:1497:GLU:O	3:N:1501:GLU:HG2	2.14	0.48
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.96	0.48
3:D:808:THR:HB	3:D:810:GLU:HG2	1.95	0.48
5:F:193:ARG:HB3	6:G:7:DG:H5''	1.94	0.48
1:L:150:TYR:CE2	1:L:170:VAL:HG22	2.49	0.48
2:M:740:GLU:HB3	2:M:805:ARG:NH1	2.29	0.47
3:N:48:ARG:NE	3:N:76:CYS:O	2.46	0.47
3:N:1130:ARG:HD2	3:N:1130:ARG:HA	1.56	0.47
1:B:106:PRO:HA	1:B:132:LEU:O	2.14	0.47
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.96	0.47
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.95	0.47
3:D:801:GLY:HA2	3:D:821:VAL:HG22	1.95	0.47
2:M:68:PHE:HA	2:M:98:LEU:HD23	1.96	0.47
2:M:189:ARG:NH1	2:M:242:LEU:HA	2.28	0.47
2:M:922:PHE:HB2	2:M:967:PHE:CD2	2.49	0.47
3:N:208:PRO:HG2	3:N:353:VAL:HG21	1.94	0.47
5:P:321:ILE:HG13	5:P:332:PHE:HE2	1.78	0.47
5:P:397:ILE:HA	5:P:400:ILE:HG22	1.95	0.47
1:A:112:ARG:HB3	1:A:125:PRO:HB3	1.95	0.47
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.95	0.47
3:D:456:MET:HE1	3:D:568:ARG:NE	2.29	0.47
2:M:643:VAL:HG11	2:M:655:LEU:HD23	1.95	0.47
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.97	0.47
3:D:800:LYS:HB3	3:D:822:ALA:H	1.78	0.47
3:D:1094:LEU:O	3:D:1098:LEU:HG	2.13	0.47
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.96	0.47
1:K:150:TYR:CE2	1:K:152:PRO:HG3	2.50	0.47
3:N:1336:LEU:HB2	3:N:1344:VAL:HG21	1.96	0.47
2:C:805:ARG:HE	2:C:807:ARG:HD3	1.79	0.47
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.48	0.47
3:N:45:PHE:HZ	3:N:541:ASN:HD21	1.62	0.47
3:N:215:TYR:HE1	3:N:381:ALA:H	1.63	0.47
1:A:31:GLY:N	1:A:193:ASP:OD2	2.47	0.47
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.97	0.47
2:C:1000:MET:O	2:C:1004:LYS:HG2	2.14	0.47
2:M:39:ARG:NH1	2:M:71:TYR:O	2.35	0.47
3:N:1101:VAL:O	3:N:1374:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:ILE:HD11	2:C:344:PHE:CE1	2.50	0.47
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.97	0.47
5:F:321:ILE:HB	5:F:327:SER:OG	2.15	0.47
2:M:541:SER:O	2:M:545:ASN:ND2	2.43	0.47
3:N:1071:PHE:O	3:N:1074:SER:OG	2.32	0.47
3:N:1288:GLU:HG3	3:N:1289:LYS:HG3	1.96	0.47
4:O:41:GLU:HB2	4:O:44:GLU:HG3	1.97	0.47
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.78	0.47
2:M:195:LEU:O	2:M:199:VAL:HG23	2.15	0.47
2:M:214:TYR:HE2	2:M:312:ALA:HA	1.80	0.47
2:M:1019:GLN:HG3	2:M:1058:ASP:HB3	1.97	0.47
5:F:129:GLU:HB3	5:F:151:LEU:HD21	1.97	0.47
1:K:175:ARG:HE	1:K:202:ASP:HB3	1.80	0.47
2:M:146:VAL:HG22	2:M:162:ILE:HG12	1.97	0.47
1:A:222:LEU:HD22	1:B:215:VAL:HG13	1.97	0.47
2:C:719:PRO:HB3	2:C:820:ARG:NE	2.30	0.47
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.50	0.47
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.96	0.47
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.96	0.47
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.15	0.46
4:E:33:HIS:NE2	4:E:89:MET:HB3	2.30	0.46
1:K:156:HIS:NE2	1:K:167:VAL:O	2.29	0.46
2:M:356:ARG:HA	2:M:359:MET:HE2	1.97	0.46
5:P:383:LEU:HA	5:P:386:VAL:HG12	1.98	0.46
7:H:14:DG:H2'	7:H:15:DC:H6	1.80	0.46
2:C:835:VAL:HG12	3:D:632:VAL:HG21	1.97	0.46
2:M:141:HIS:HE1	2:M:332:ARG:HH11	1.63	0.46
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.95	0.46
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.98	0.46
3:N:1190:SER:OG	3:N:1369:GLU:OE1	2.27	0.46
5:P:152:ASP:O	5:P:156:VAL:HG13	2.15	0.46
3:D:411:THR:O	5:F:178:ARG:NH1	2.42	0.46
2:M:682:TYR:HA	3:N:633:VAL:HG11	1.98	0.46
3:N:100:ALA:HA	3:N:513:ILE:HG13	1.97	0.46
3:N:570:GLU:OE2	5:P:214:GLN:NE2	2.44	0.46
3:N:1144:LEU:O	3:N:1147:ARG:HG3	2.16	0.46
2:C:48:PHE:CD1	2:C:348:LEU:HD21	2.51	0.46
2:C:648:ARG:HH11	2:C:648:ARG:HB3	1.80	0.46
3:D:214:GLU:OE1	3:D:342:PRO:HB3	2.16	0.46
2:M:1001:VAL:HG22	3:N:630:VAL:HB	1.96	0.46
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:573:MET:SD	5:F:210:LEU:HB3	2.54	0.46
1:L:124:ASN:OD1	1:L:124:ASN:N	2.48	0.46
1:L:172:SER:OG	1:L:174:VAL:O	2.33	0.46
2:M:1019:GLN:HE22	3:N:617:ASN:HB3	1.81	0.46
3:N:1089:ALA:HA	7:Q:14:DG:C8	2.50	0.46
5:P:412:GLU:HA	5:P:415:THR:HG22	1.97	0.46
3:N:5:VAL:O	3:N:1470:ARG:NH2	2.48	0.46
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.51	0.46
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.97	0.46
3:N:804:LEU:O	3:N:827:ILE:HG13	2.16	0.46
3:N:1310:ARG:HB2	3:N:1327:ARG:HB2	1.97	0.46
3:N:1458:GLU:HB2	3:N:1460:ILE:HD13	1.97	0.46
5:P:93:LEU:HD21	5:P:193:ARG:HD2	1.96	0.46
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.50	0.46
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.46	0.46
2:M:185:LYS:HA	2:M:189:ARG:O	2.16	0.46
2:M:598:GLU:O	2:M:651:LYS:HG3	2.15	0.46
2:M:1097:LEU:HD11	3:N:103:TRP:HZ3	1.81	0.46
7:H:6:DA:H2'	7:H:7:DT:H71	1.98	0.46
1:A:24:VAL:HA	1:A:195:LEU:O	2.16	0.46
2:C:535:SER:O	2:C:538:GLN:HG2	2.16	0.46
3:D:231:VAL:O	3:D:236:TYR:OH	2.34	0.46
2:M:1016:ILE:O	3:N:87:ARG:NH1	2.48	0.46
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.98	0.46
3:N:614:PHE:HA	3:N:618:LEU:HD12	1.96	0.46
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.31	0.46
2:C:1058:ASP:OD2	3:D:621:LYS:HE3	2.16	0.46
3:D:361:VAL:O	3:D:382:GLU:HA	2.15	0.46
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.96	0.46
1:K:104:GLU:HG2	1:K:137:ARG:HG2	1.98	0.46
2:C:637:LEU:HA	2:C:659:PRO:HG3	1.98	0.45
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.98	0.45
3:D:895:VAL:O	3:D:899:LEU:HG	2.16	0.45
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.51	0.45
2:M:940:GLU:HG2	2:M:973:VAL:HG21	1.98	0.45
2:M:1005:MET:HE1	3:N:647:ARG:HB3	1.97	0.45
3:N:1094:LEU:O	3:N:1098:LEU:HG	2.16	0.45
5:P:401:GLU:HG2	5:P:402:ASN:N	2.28	0.45
2:C:670:GLN:OE1	2:C:700:TYR:N	2.48	0.45
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.97	0.45
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:ARG:HH21	1:L:192:LEU:HD21	1.81	0.45
2:M:237:ARG:O	2:M:241:LEU:HG	2.17	0.45
2:M:709:GLU:HG3	2:M:824:ARG:HG2	1.98	0.45
3:N:1496:GLU:O	3:N:1499:ARG:HG2	2.16	0.45
6:G:18:DC:H2''	6:G:19:DG:H8	1.80	0.45
3:D:166:GLN:HB2	3:D:394:LEU:HD11	1.98	0.45
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.97	0.45
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.64	0.45
2:M:657:ASP:OD2	2:M:663:ASN:N	2.42	0.45
3:N:610:LYS:HD2	7:Q:15:DC:OP1	2.16	0.45
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.51	0.45
3:N:895:VAL:O	3:N:899:LEU:HG	2.17	0.45
3:N:1383:ASP:HB3	3:N:1416:ALA:HB3	1.99	0.45
3:D:200:ASP:N	3:D:200:ASP:OD1	2.48	0.45
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.51	0.45
2:M:1090:LYS:HA	2:M:1090:LYS:HD3	1.78	0.45
3:N:471:GLU:H	3:N:471:GLU:HG2	1.44	0.45
1:B:153:ALA:HB1	1:B:166:PRO:HB2	1.98	0.45
2:C:251:ASP:OD1	2:C:251:ASP:N	2.39	0.45
3:D:1127:GLU:CD	3:D:1127:GLU:H	2.25	0.45
1:K:53:VAL:HG22	1:K:144:VAL:HG22	1.98	0.45
1:L:150:TYR:HE2	1:L:170:VAL:HG22	1.80	0.45
2:M:250:ARG:CZ	2:M:250:ARG:HB3	2.45	0.45
2:M:731:GLU:HA	2:M:734:LEU:HD12	1.96	0.45
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.51	0.45
2:C:631:SER:HB3	2:C:637:LEU:HG	1.97	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.45
2:M:235:LEU:HD21	2:M:254:VAL:HG23	1.99	0.45
2:M:344:PHE:HD1	2:M:382:ILE:HD11	1.80	0.45
2:M:584:GLU:CD	2:M:584:GLU:H	2.23	0.45
3:N:573:MET:SD	5:P:210:LEU:HB3	2.56	0.45
6:J:11:DG:H2'	6:J:12:DC:C5	2.52	0.45
1:A:11:PHE:O	1:B:228:PRO:HA	2.17	0.45
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.52	0.45
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.52	0.45
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.24	0.45
2:M:939:ARG:H	2:M:939:ARG:HG2	1.40	0.45
3:N:62:LYS:HB3	11:N:1704:HOH:O	2.16	0.45
3:N:959:GLU:OE1	3:N:959:GLU:N	2.41	0.45
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.52	0.45
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1040:GLY:O	3:N:1060:SER:HB3	2.16	0.45
1:A:66:SER:HB2	1:A:75:VAL:HG21	1.99	0.45
2:C:582:GLY:N	2:C:584:GLU:OE2	2.47	0.45
1:K:58:ILE:HG12	1:K:140:MET:HB3	1.99	0.45
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.24	0.45
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.99	0.45
2:M:3:ILE:HD13	2:M:900:ARG:HB2	1.98	0.45
7:Q:4:DG:H2'	7:Q:5:DC:C6	2.52	0.45
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.82	0.44
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.98	0.44
3:D:1161:GLU:CD	3:D:1164:ARG:HB2	2.42	0.44
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.98	0.44
2:M:17:PRO:HB2	2:M:20:GLU:HB3	1.99	0.44
4:O:13:VAL:HG21	4:O:19:LEU:HB2	1.98	0.44
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.98	0.44
3:D:73:CYS:HB3	3:D:76:CYS:SG	2.56	0.44
5:F:386:VAL:HG12	5:F:397:ILE:HD12	1.99	0.44
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.52	0.44
1:L:132:LEU:HD21	1:L:138:LEU:HB2	1.99	0.44
2:M:105:THR:HG22	2:M:107:LEU:H	1.82	0.44
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	2.00	0.44
3:N:141:ILE:HA	3:N:146:PRO:HA	1.98	0.44
2:C:351:LEU:HD12	2:C:375:SER:HA	1.99	0.44
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.53	0.44
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.99	0.44
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.99	0.44
3:N:526:PRO:HB2	3:N:528:VAL:HG13	1.98	0.44
2:C:259:GLY:HA2	2:C:263:ASP:HB2	2.00	0.44
5:F:166:LEU:HB3	5:F:170:HIS:HB2	2.00	0.44
2:M:1009:SER:O	3:N:624:ASP:HB3	2.18	0.44
3:N:352:ASN:OD1	3:N:352:ASN:N	2.50	0.44
3:N:586:ARG:HD2	3:N:586:ARG:HA	1.80	0.44
7:Q:9:DC:H2''	7:Q:10:DG:H8	1.82	0.44
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.52	0.44
1:B:91:ASN:HB3	1:B:94:LEU:HB2	2.00	0.44
2:C:436:GLY:HA2	2:C:538:GLN:O	2.18	0.44
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.98	0.44
3:D:711:LEU:HD13	3:D:778:LEU:HD11	2.00	0.44
2:M:880:MET:HA	3:N:1038:LEU:HD21	2.00	0.44
1:A:133:GLU:HG2	1:A:134:GLU:N	2.32	0.44
2:C:74:GLY:HA3	2:C:93:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASN:O	2:C:884:GLN:HG2	2.17	0.44
3:D:300:LYS:HE3	3:D:300:LYS:HB2	1.83	0.44
3:D:886:VAL:O	3:D:890:VAL:HG22	2.18	0.44
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.53	0.44
2:M:805:ARG:NH2	2:M:821:GLU:OE1	2.51	0.44
3:N:101:HIS:CE1	3:N:582:LEU:HD13	2.52	0.44
7:Q:5:DC:H2'	7:Q:6:DA:C8	2.52	0.44
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.79	0.44
3:D:1406:ARG:O	3:D:1410:GLU:HB2	2.18	0.44
5:F:384:GLU:OE2	5:F:394:ARG:NE	2.48	0.44
3:N:15:PRO:O	3:N:19:ARG:HG3	2.18	0.44
3:N:296:GLU:HG3	3:N:297:ILE:N	2.33	0.44
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.75	0.44
1:L:83:LYS:HE2	1:L:168:ASP:HB2	2.00	0.44
2:M:896:PHE:HB2	2:M:921:ALA:HB1	2.00	0.44
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.00	0.44
3:D:214:GLU:HB3	3:D:340:THR:HB	2.00	0.44
3:D:1130:ARG:HA	3:D:1130:ARG:HD3	1.70	0.44
5:F:392:VAL:HG23	5:F:397:ILE:HG12	2.00	0.44
2:M:191:PHE:CZ	2:M:238:LEU:HD11	2.52	0.44
3:N:223:LEU:HD11	3:N:288:MET:HE1	2.00	0.44
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.53	0.44
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.88	0.43
1:A:73:GLU:N	1:A:73:GLU:OE1	2.50	0.43
1:A:184:THR:O	1:A:192:LEU:HB2	2.18	0.43
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.00	0.43
2:C:134:ARG:HH12	2:C:392:SER:C	2.26	0.43
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	2.00	0.43
3:D:288:MET:HE2	3:D:288:MET:HB3	1.91	0.43
3:D:828:LYS:HA	3:D:833:GLU:HA	1.99	0.43
3:D:1258:ARG:NH1	3:D:1261:GLU:OE2	2.45	0.43
3:D:1289:LYS:HG2	3:D:1290:LEU:H	1.82	0.43
2:M:191:PHE:HB2	2:M:192:PRO:HD2	2.00	0.43
3:N:156:GLU:CD	3:N:156:GLU:H	2.26	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.75	0.43
4:E:66:LYS:O	4:E:70:THR:HG23	2.17	0.43
5:F:372:ARG:HG2	5:F:386:VAL:HG21	2.00	0.43
2:M:561:GLY:O	2:M:565:GLN:HG3	2.18	0.43
2:M:578:VAL:HG13	2:M:671:ASN:CG	2.43	0.43
3:N:181:ASP:HB2	3:N:205:TYR:CD2	2.52	0.43
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:567:ILE:HG22	3:N:571:LYS:HE3	2.00	0.43
3:N:638:LYS:HA	3:N:638:LYS:HD3	1.88	0.43
5:P:383:LEU:HD11	5:P:398:ARG:HD3	1.99	0.43
2:C:496:ILE:HG12	2:C:531:PHE:HB2	2.00	0.43
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.49	0.43
1:L:44:LEU:O	1:L:174:VAL:HG11	2.19	0.43
2:M:195:LEU:HG	2:M:238:LEU:HB2	2.01	0.43
3:N:783:ARG:H	3:N:783:ARG:HG2	1.32	0.43
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.33	0.43
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	1.99	0.43
5:P:364:ARG:O	5:P:368:VAL:HG13	2.18	0.43
2:C:6:PHE:CE1	2:C:909:ALA:HB2	2.54	0.43
2:C:226:VAL:HA	2:C:229:MET:HE3	2.00	0.43
2:C:944:LEU:HD21	2:C:963:LEU:HD23	2.00	0.43
3:D:959:GLU:OE1	3:D:959:GLU:N	2.50	0.43
2:M:374:ASN:OD1	5:P:276:ARG:HD3	2.17	0.43
2:M:677:MET:SD	2:M:987:ILE:HD13	2.59	0.43
3:N:214:GLU:OE1	3:N:342:PRO:HB3	2.19	0.43
3:N:881:LEU:O	3:N:885:ILE:HG13	2.18	0.43
3:N:1236:LEU:HD22	3:N:1355:VAL:HG12	2.00	0.43
3:D:215:TYR:HE2	3:D:381:ALA:H	1.66	0.43
3:D:218:LYS:HG2	3:D:338:GLU:HG2	2.00	0.43
3:D:638:LYS:HA	3:D:638:LYS:HD3	1.82	0.43
5:P:201:LYS:NZ	5:P:244:ARG:HH21	2.17	0.43
1:B:101:LEU:HB2	1:B:114:PHE:CD1	2.53	0.43
2:C:1020:PRO:HD2	3:D:622:ARG:O	2.19	0.43
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.00	0.43
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.54	0.43
1:L:56:VAL:HG22	1:L:142:VAL:HG12	2.01	0.43
2:M:402:SER:HA	2:M:566:THR:HG23	2.01	0.43
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.99	0.43
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	2.01	0.43
3:N:1278:ASP:HA	3:N:1319:VAL:O	2.19	0.43
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.53	0.43
1:B:80:LEU:HD21	3:D:842:VAL:HG12	2.00	0.43
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.00	0.43
3:D:703:ASN:HB2	3:D:713:ILE:HG12	2.00	0.43
5:F:152:ASP:OD1	5:F:152:ASP:N	2.49	0.43
1:K:230:ALA:HA	1:L:13:VAL:O	2.18	0.43
3:N:268:ALA:HB3	3:N:284:LEU:HD12	2.00	0.43
3:N:783:ARG:HB3	3:N:1028:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HB3	1:A:125:PRO:HA	1.99	0.43
3:D:770:LEU:HA	3:D:777:PRO:HA	1.99	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
4:O:42:PRO:HA	4:O:45:ARG:HD2	2.00	0.43
2:C:358:ARG:HH22	2:C:374:ASN:HD22	1.66	0.43
3:D:274:ARG:NH1	3:D:279:VAL:HG21	2.34	0.43
3:D:574:LEU:O	3:D:578:VAL:HG23	2.18	0.43
4:E:83:ASP:OD1	4:E:83:ASP:N	2.52	0.43
5:F:279:GLN:HG3	5:F:280:GLN:N	2.34	0.43
2:M:765:SER:O	2:M:767:PRO:HD3	2.19	0.43
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.85	0.43
1:L:77:GLU:O	1:L:81:ASN:ND2	2.50	0.43
1:L:174:VAL:HA	1:L:201:THR:HA	2.01	0.43
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.54	0.43
2:C:588:VAL:HG13	2:C:593:ALA:HB3	2.00	0.42
2:C:905:ILE:HG23	2:C:906:PHE:CD2	2.49	0.42
3:D:1000:THR:HG23	3:D:1036:ARG:HD2	2.00	0.42
5:F:101:GLU:HG3	5:F:105:LYS:HE2	2.01	0.42
1:L:153:ALA:HA	1:L:156:HIS:NE2	2.33	0.42
2:M:367:LEU:HD13	2:M:372:LEU:HD11	2.00	0.42
3:N:1487:VAL:HG22	3:N:1491:THR:HB	2.01	0.42
5:P:404:ALA:O	5:P:408:LEU:HB2	2.18	0.42
3:D:782:SER:OG	3:D:783:ARG:HG2	2.18	0.42
2:M:462:ASP:OD1	2:M:466:PHE:N	2.49	0.42
3:N:658:LEU:HB3	3:N:670:VAL:HG13	2.02	0.42
2:C:163:ILE:HG23	2:C:171:TRP:NE1	2.34	0.42
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.59	0.42
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.54	0.42
3:D:661:MET:HE1	3:D:677:LEU:HD11	2.02	0.42
1:K:68:ILE:H	1:K:68:ILE:HG13	1.60	0.42
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.54	0.42
2:M:589:ARG:HD3	2:M:596:TYR:CE1	2.55	0.42
2:M:850:ALA:HB1	3:N:633:VAL:HG12	2.02	0.42
3:N:563:PRO:HD2	3:N:566:ILE:HD12	2.00	0.42
3:N:622:ARG:NH1	7:Q:17:DT:OP1	2.52	0.42
3:N:661:MET:HE3	3:N:673:ALA:HB1	2.02	0.42
3:N:1461:GLY:O	3:N:1465:ASN:ND2	2.52	0.42
1:A:100:LEU:HD23	1:A:141:GLU:HG2	2.00	0.42
3:D:65:ARG:HB3	3:D:67:ARG:HG3	2.01	0.42
3:D:415:VAL:HG13	3:D:419:ASP:HB2	2.01	0.42
2:M:437:ARG:NH1	2:M:491:GLU:OE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:LEU:HD11	2:C:373:VAL:HG13	2.02	0.42
3:D:563:PRO:HD2	3:D:566:ILE:HD12	2.01	0.42
5:F:207:LEU:HD21	5:F:254:GLN:HB2	2.00	0.42
1:L:54:THR:HG22	1:L:156:HIS:CE1	2.54	0.42
2:M:9:ILE:HD11	2:M:500:ASN:HA	1.99	0.42
2:M:74:GLY:HA3	2:M:93:PRO:HG2	2.01	0.42
3:N:132:TYR:O	3:N:152:LEU:HA	2.20	0.42
3:N:654:LYS:O	3:N:658:LEU:HG	2.20	0.42
2:C:440:PRO:HB2	3:D:1074:SER:HB2	2.02	0.42
2:C:714:ASP:OD1	2:C:820:ARG:NE	2.52	0.42
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.93	0.42
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.00	0.42
3:D:618:LEU:HD13	3:D:1467:ILE:HG23	2.00	0.42
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.34	0.42
1:L:58:ILE:HG12	1:L:140:MET:HE2	2.01	0.42
2:M:124:ASP:HB3	2:M:592:LEU:HD12	2.02	0.42
2:M:878:SER:HA	3:N:1034:GLN:OE1	2.19	0.42
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.36	0.42
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.18	0.42
5:P:287:THR:OG1	5:P:290:GLU:HG3	2.19	0.42
1:L:115:LEU:HA	1:L:116:PRO:HD3	1.95	0.42
2:M:30:LEU:HD22	2:M:73:LEU:HD11	2.02	0.42
2:M:503:LEU:HD23	2:M:508:ILE:HA	2.00	0.42
3:N:44:LEU:O	3:N:525:ARG:NH2	2.39	0.42
3:N:136:ASP:HB3	3:N:453:ASP:HB3	1.99	0.42
5:P:407:LYS:HD3	5:P:407:LYS:HA	1.78	0.42
7:H:4:DG:H2'	7:H:5:DC:C6	2.54	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.87	0.42
1:A:111:ALA:HB2	1:A:127:LEU:HB3	2.02	0.42
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.55	0.42
3:D:45:PHE:O	3:D:86:ARG:NH2	2.53	0.42
3:D:367:ILE:HB	3:D:377:VAL:HG12	2.02	0.42
3:D:1216:SER:HB3	4:E:15:SER:HA	2.02	0.42
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.02	0.42
3:N:1331:ASP:HB3	3:N:1334:GLN:HB2	2.00	0.42
2:C:680:ASP:H	3:D:943:THR:HG22	1.85	0.42
1:K:198:ARG:HH22	2:M:932:GLU:CD	2.28	0.42
1:K:218:LEU:HG	1:L:222:LEU:HD11	2.02	0.42
2:M:385:PHE:O	2:M:389:SER:CB	2.67	0.42
2:M:400:PRO:HB3	2:M:591:SER:HB3	2.02	0.42
2:M:468:ARG:NE	2:M:487:THR:HG23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:LEU:HD21	2:C:237:ARG:HG3	2.01	0.42
2:C:328:LEU:HD12	2:C:433:THR:O	2.20	0.42
2:C:1057:SER:OG	2:C:1058:ASP:N	2.53	0.42
3:D:310:LEU:H	3:D:310:LEU:HD12	1.85	0.42
2:M:230:ARG:HB2	2:M:231:PRO:HD2	2.02	0.42
2:M:251:ASP:OD1	2:M:251:ASP:N	2.50	0.42
2:M:708:TYR:HB3	2:M:790:LEU:HD21	2.02	0.42
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	2.02	0.42
3:N:363:ALA:HB2	3:N:381:ALA:HA	2.01	0.42
3:N:684:LYS:HD3	3:N:686:GLU:OE1	2.20	0.42
5:P:373:LYS:HA	5:P:373:LYS:HD3	1.83	0.42
1:A:79:ILE:O	1:A:83:LYS:HG3	2.20	0.41
3:D:355:VAL:HG13	3:D:359:ALA:HB3	2.02	0.41
5:F:172:ARG:O	5:F:176:ILE:HG12	2.20	0.41
1:K:183:ASP:OD1	1:K:191:ASP:HA	2.20	0.41
3:N:206:ARG:HA	3:N:206:ARG:HH11	1.85	0.41
3:N:841:TYR:HB2	3:N:864:VAL:HG22	2.02	0.41
3:N:1046:GLN:N	3:N:1046:GLN:OE1	2.53	0.41
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.02	0.41
2:M:30:LEU:HD23	2:M:30:LEU:HA	1.87	0.41
2:M:139:GLN:HB2	2:M:391:LEU:HD11	2.01	0.41
2:M:215:GLY:O	2:M:216:GLU:CB	2.69	0.41
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.20	0.41
3:N:1122:LEU:HD13	3:N:1178:ALA:HB2	2.02	0.41
3:N:1161:GLU:CD	3:N:1164:ARG:HB2	2.44	0.41
2:C:687:ALA:HB1	2:C:850:ALA:HB2	2.02	0.41
2:C:693:GLU:CD	2:C:696:LYS:HD2	2.45	0.41
2:C:830:LYS:HE2	2:C:830:LYS:HB3	1.80	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HH12	1.84	0.41
3:D:783:ARG:HD2	3:D:1029:ARG:HG2	2.02	0.41
1:L:59:GLU:HB2	1:L:139:ASN:HB3	2.02	0.41
1:L:108:GLU:HG2	1:L:131:THR:HG22	2.02	0.41
2:M:36:PRO:HA	2:M:39:ARG:HD2	2.03	0.41
2:M:41:ASN:C	2:M:46:ALA:HB2	2.46	0.41
3:N:209:ARG:O	3:N:346:ARG:HD3	2.20	0.41
3:N:227:LEU:HD13	3:N:331:VAL:HG13	2.03	0.41
1:A:220:GLU:O	1:A:223:THR:HB	2.20	0.41
1:B:26:GLU:HA	1:B:27:PRO:HA	1.93	0.41
2:C:580:MET:HB3	2:C:584:GLU:CD	2.45	0.41
5:F:95:THR:HB	5:F:98:GLU:HG3	2.02	0.41
2:M:1054:THR:O	2:M:1059:ASP:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:411:THR:HB	3:N:437:VAL:H	1.85	0.41
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.85	0.41
3:N:561:GLY:HA3	5:P:132:ARG:HD3	2.02	0.41
3:N:806:PHE:CE1	3:N:827:ILE:HD11	2.55	0.41
4:O:46:PRO:HD2	4:O:63:TRP:CE2	2.56	0.41
1:A:218:LEU:HG	1:B:222:LEU:HD11	2.02	0.41
3:D:401:TYR:HB3	3:D:427:VAL:HG21	2.03	0.41
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.59	0.41
1:K:9:PRO:CB	1:K:27:PRO:HD2	2.48	0.41
1:K:103:ALA:HB1	1:K:107:LYS:HD3	2.02	0.41
2:M:163:ILE:HG23	2:M:171:TRP:NE1	2.36	0.41
2:M:1070:ILE:CG2	3:N:655:PRO:HB2	2.51	0.41
2:C:206:THR:HA	2:C:209:ARG:HG2	2.03	0.41
2:C:715:THR:HB	2:C:717:LEU:H	1.85	0.41
1:L:64:GLU:HA	1:L:165:ILE:HD13	2.01	0.41
2:M:564:MET:SD	2:M:846:LYS:HD3	2.60	0.41
2:M:734:LEU:HB3	2:M:737:LEU:HD12	2.02	0.41
7:H:12:DG:H2'	7:H:13:DA:C8	2.56	0.41
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.03	0.41
2:C:425:PHE:CE2	3:D:1079:LYS:HE3	2.55	0.41
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.53	0.41
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.85	0.41
5:F:193:ARG:HB2	6:G:6:DT:H1'	2.03	0.41
2:M:154:ARG:HA	2:M:155:PRO:HD3	1.85	0.41
2:M:261:ILE:HD11	2:M:303:PHE:HZ	1.85	0.41
3:N:731:LEU:HD23	3:N:731:LEU:HA	1.92	0.41
3:N:908:LYS:HB3	3:N:908:LYS:HE2	1.82	0.41
3:N:1465:ASN:HB3	3:N:1470:ARG:HB2	2.01	0.41
1:A:54:THR:HG21	1:A:145:ASP:HB2	2.02	0.41
3:D:842:VAL:HG22	3:D:865:THR:HB	2.02	0.41
3:D:1098:LEU:HA	3:D:1101:VAL:HG12	2.02	0.41
2:M:860:HIS:CE1	2:M:975:TYR:HB2	2.56	0.41
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.85	0.41
3:N:539:ASP:OD2	3:N:598:ARG:NH1	2.50	0.41
3:N:540:LEU:HD23	3:N:543:LEU:HD12	2.03	0.41
3:N:1236:LEU:HD13	3:N:1259:VAL:HG21	2.02	0.41
1:A:101:LEU:HD13	1:A:140:MET:HE3	2.02	0.41
1:A:133:GLU:HG3	2:C:645:VAL:HG21	2.03	0.41
1:A:176:ARG:HG3	1:A:177:VAL:N	2.35	0.41
2:C:210:GLU:HG2	2:C:304:LEU:HD21	2.02	0.41
2:C:563:ASN:O	2:C:566:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.56	0.41
3:D:95:LEU:HD22	3:D:574:LEU:HD21	2.03	0.41
3:D:534:ARG:HE	3:D:534:ARG:HB3	1.63	0.41
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.56	0.41
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.53	0.41
1:K:41:ARG:HA	1:K:177:VAL:HG11	2.01	0.41
3:N:134:VAL:HG23	3:N:149:LYS:HA	2.03	0.41
3:N:236:TYR:CZ	3:N:242:LEU:HD12	2.56	0.41
5:P:153:PRO:HA	5:P:156:VAL:HG22	2.01	0.41
5:P:399:GLN:O	5:P:403:LYS:HG2	2.21	0.41
7:H:11:DT:H2"	7:H:12:DG:C8	2.55	0.41
2:C:895:TYR:HB2	2:C:991:GLN:HG3	2.03	0.41
3:D:353:VAL:HG12	3:D:355:VAL:H	1.85	0.41
2:M:210:GLU:HG2	2:M:304:LEU:HD21	2.03	0.41
1:B:213:GLN:O	1:B:217:ILE:HG13	2.21	0.40
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.03	0.40
2:C:861:LEU:HD12	2:C:865:THR:HB	2.03	0.40
3:D:956:ILE:HD13	3:D:1039:CYS:O	2.21	0.40
1:K:108:GLU:HG2	1:K:131:THR:HG23	2.02	0.40
2:M:28:ARG:NH1	2:M:42:VAL:HG11	2.36	0.40
2:M:195:LEU:HD21	2:M:237:ARG:HG3	2.01	0.40
2:M:328:LEU:HA	2:M:328:LEU:HD23	1.79	0.40
2:M:401:LEU:HD13	2:M:587:VAL:HG11	2.03	0.40
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.31	0.40
3:N:477:LEU:HB2	3:N:496:LEU:HD13	2.04	0.40
3:N:1453:ALA:HB3	3:N:1455:LYS:HG3	2.03	0.40
5:P:141:VAL:O	5:P:142:ARG:HG3	2.20	0.40
1:A:16:GLN:HB2	1:A:20:TYR:HB3	2.03	0.40
1:A:64:GLU:HG3	1:A:79:ILE:HD12	2.03	0.40
1:A:183:ASP:HA	2:C:938:LYS:HE3	2.03	0.40
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.35	0.40
2:C:1042:ALA:HA	3:D:1220:ALA:HB3	2.02	0.40
3:D:897:TRP:HA	3:D:900:ILE:HD12	2.03	0.40
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.20	0.40
4:E:87:LYS:HA	4:E:87:LYS:HD3	1.91	0.40
5:F:181:GLU:O	5:F:185:GLN:HG2	2.21	0.40
1:K:220:GLU:O	1:K:223:THR:HB	2.21	0.40
2:M:344:PHE:CD1	2:M:382:ILE:HD11	2.56	0.40
2:C:328:LEU:HA	2:C:328:LEU:HD23	1.83	0.40
3:D:236:TYR:HD2	3:D:322:VAL:HG21	1.86	0.40
3:N:8:VAL:HG12	3:N:1434:TRP:HZ2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:633:VAL:HA	3:N:740:PHE:CZ	2.56	0.40
3:N:1488:ASP:OD1	3:N:1488:ASP:N	2.48	0.40
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.56	0.40
1:B:211:LEU:O	1:B:215:VAL:HG23	2.22	0.40
2:C:66:LEU:HD11	2:C:98:LEU:HB3	2.04	0.40
2:C:589:ARG:NH2	2:C:652:GLY:O	2.49	0.40
2:C:680:ASP:OD1	3:D:943:THR:HG21	2.22	0.40
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	2.04	0.40
3:D:1216:SER:OG	4:E:16:LYS:HG2	2.21	0.40
2:M:69:LEU:HD21	2:M:99:GLN:CD	2.46	0.40
2:M:214:TYR:CE2	2:M:312:ALA:HA	2.55	0.40
2:M:712:ALA:HB3	2:M:821:GLU:HG3	2.02	0.40
3:N:127:LEU:HA	3:N:457:GLY:HA2	2.02	0.40
3:N:255:GLU:HA	3:N:300:LYS:HE2	2.03	0.40
3:N:1485:GLN:NE2	4:O:82:GLU:OE1	2.55	0.40
5:P:234:LYS:HB3	5:P:234:LYS:HE2	1.87	0.40
1:A:176:ARG:HG2	1:A:200:TRP:CE3	2.55	0.40
1:A:201:THR:HG22	1:A:203:GLY:H	1.85	0.40
2:C:224:GLU:CD	2:C:224:GLU:H	2.28	0.40
2:M:236:ILE:HG23	2:M:248:PRO:HB2	2.02	0.40
3:N:943:THR:OG1	3:N:944:THR:N	2.55	0.40
3:N:1126:ASP:OD1	3:N:1126:ASP:N	2.47	0.40
3:N:1383:ASP:HA	3:N:1384:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	5/315 (2%)	5 (100%)	0	0	100	100
1	B	86/315 (27%)	83 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	225/315 (71%)	219 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	219 (98%)	4 (2%)	0	100	100
2	C	1107/1119 (99%)	1082 (98%)	25 (2%)	0	100	100
2	M	1107/1119 (99%)	1077 (97%)	30 (3%)	0	100	100
3	D	1482/1524 (97%)	1447 (98%)	35 (2%)	0	100	100
3	N	1482/1524 (97%)	1446 (98%)	36 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
4	O	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	342 (99%)	2 (1%)	0	100	100
5	P	345/443 (78%)	334 (97%)	11 (3%)	0	100	100
All	All	6590/7630 (86%)	6435 (98%)	155 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/273 (71%)	178 (91%)	17 (9%)	9	33
1	B	195/273 (71%)	178 (91%)	17 (9%)	9	33
1	K	198/273 (72%)	181 (91%)	17 (9%)	10	34
1	L	198/273 (72%)	186 (94%)	12 (6%)	17	46
2	C	931/941 (99%)	865 (93%)	66 (7%)	13	41
2	M	927/941 (98%)	860 (93%)	67 (7%)	13	40
3	D	1241/1279 (97%)	1161 (94%)	80 (6%)	16	44
3	N	1240/1279 (97%)	1161 (94%)	79 (6%)	16	44
4	E	83/88 (94%)	79 (95%)	4 (5%)	23	52
4	O	83/88 (94%)	79 (95%)	4 (5%)	23	52
5	F	300/388 (77%)	283 (94%)	17 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	291/388 (75%)	273 (94%)	18 (6%)	16	45
All	All	5882/6484 (91%)	5484 (93%)	398 (7%)	14	43

All (398) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	10	VAL
1	A	24	VAL
1	A	34	VAL
1	A	36	LEU
1	A	67	THR
1	A	76	VAL
1	A	90	LEU
1	A	100	LEU
1	A	134	GLU
1	A	142	VAL
1	A	148	VAL
1	A	184	THR
1	A	188	GLN
1	A	205	VAL
1	A	206	THR
1	A	229	GLN
1	B	7	LYS
1	B	10	VAL
1	B	12	THR
1	B	34	VAL
1	B	38	ASN
1	B	56	VAL
1	B	66	SER
1	B	96	THR
1	B	113	ASP
1	B	124	ASN
1	B	133	GLU
1	B	142	VAL
1	B	186	LEU
1	B	188	GLN
1	B	190	THR
1	B	197	LEU
1	B	205	VAL
2	C	1	MET
2	C	21	ILE

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Mol	Chain	Res	Type
2	C	50	GLU
2	C	133	ASP
2	C	138	SER
2	C	149	THR
2	C	159	ILE
2	C	177	GLU
2	C	182	VAL
2	C	194	VAL
2	C	196	LEU
2	C	206	THR
2	C	218	VAL
2	C	221	LEU
2	C	224	GLU
2	C	251	ASP
2	C	261	ILE
2	C	321	GLU
2	C	335	THR
2	C	346	VAL
2	C	365	ASP
2	C	402	SER
2	C	419	THR
2	C	429	ASP
2	C	442	GLU
2	C	443	THR
2	C	453	THR
2	C	460	ARG
2	C	461	VAL
2	C	475	VAL
2	C	480	THR
2	C	482	GLU
2	C	490	GLU
2	C	504	GLU
2	C	513	VAL
2	C	524	VAL
2	C	559	LEU
2	C	560	MET
2	C	575	GLN
2	C	584	GLU
2	C	617	ASP
2	C	640	ARG
2	C	648	ARG
2	C	672	VAL

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Mol	Chain	Res	Type
2	C	683	ASN
2	C	705	ILE
2	C	715	THR
2	C	764	GLU
2	C	775	ARG
2	C	805	ARG
2	C	807	ARG
2	C	808	ARG
2	C	822	VAL
2	C	831	ARG
2	C	846	LYS
2	C	848	VAL
2	C	887	GLU
2	C	905	ILE
2	C	910	LYS
2	C	916	GLU
2	C	939	ARG
2	C	1001	VAL
2	C	1010	THR
2	C	1056	LYS
2	C	1076	VAL
2	C	1080	SER
3	D	12	LEU
3	D	17	LYS
3	D	67	ARG
3	D	68	PHE
3	D	72	VAL
3	D	80	VAL
3	D	106	LYS
3	D	115	LEU
3	D	134	VAL
3	D	171	LEU
3	D	184	GLU
3	D	185	VAL
3	D	186	VAL
3	D	200	ASP
3	D	231	VAL
3	D	241	ILE
3	D	247	GLU
3	D	256	GLU
3	D	270	LEU
3	D	275	GLU

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Mol	Chain	Res	Type
3	D	277	GLU
3	D	286	VAL
3	D	310	LEU
3	D	331	VAL
3	D	362	GLU
3	D	400	VAL
3	D	407	VAL
3	D	415	VAL
3	D	421	LEU
3	D	500	ARG
3	D	514	LEU
3	D	525	ARG
3	D	537	THR
3	D	576	GLU
3	D	586	ARG
3	D	587	ARG
3	D	647	ARG
3	D	666	ILE
3	D	669	ASN
3	D	686	GLU
3	D	687	VAL
3	D	694	VAL
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	783	ARG
3	D	805	GLU
3	D	808	THR
3	D	827	ILE
3	D	864	VAL
3	D	873	LEU
3	D	875	THR
3	D	907	GLU
3	D	940	THR
3	D	943	THR
3	D	956	ILE
3	D	1029	ARG
3	D	1055	VAL
3	D	1062	ARG
3	D	1067	VAL
3	D	1073	SER
3	D	1079	LYS

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Mol	Chain	Res	Type
3	D	1128	VAL
3	D	1130	ARG
3	D	1152	GLU
3	D	1155	VAL
3	D	1188	VAL
3	D	1216	SER
3	D	1221	VAL
3	D	1253	THR
3	D	1277	ILE
3	D	1278	ASP
3	D	1283	ILE
3	D	1326	THR
3	D	1344	VAL
3	D	1408	ILE
3	D	1422	MET
3	D	1460	ILE
3	D	1481	VAL
3	D	1486	VAL
4	E	50	THR
4	E	52	GLU
4	E	74	VAL
4	E	90	GLU
5	F	88	ILE
5	F	120	THR
5	F	135	ILE
5	F	208	SER
5	F	218	GLN
5	F	258	ILE
5	F	262	VAL
5	F	267	THR
5	F	279	GLN
5	F	326	ASP
5	F	327	SER
5	F	338	LEU
5	F	363	GLU
5	F	392	VAL
5	F	396	ARG
5	F	406	ARG
5	F	422	LEU
1	K	6	LEU
1	K	10	VAL
1	K	24	VAL

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Mol	Chain	Res	Type
1	K	25	LEU
1	K	34	VAL
1	K	67	THR
1	K	68	ILE
1	K	74	ASP
1	K	80	LEU
1	K	112	ARG
1	K	134	GLU
1	K	142	VAL
1	K	180	GLN
1	K	196	THR
1	K	205	VAL
1	K	206	THR
1	K	218	LEU
1	L	7	LYS
1	L	22	GLU
1	L	34	VAL
1	L	38	ASN
1	L	54	THR
1	L	56	VAL
1	L	93	SER
1	L	96	THR
1	L	142	VAL
1	L	172	SER
1	L	179	PHE
1	L	206	THR
2	M	1	MET
2	M	12	VAL
2	M	28	ARG
2	M	34	VAL
2	M	85	GLU
2	M	103	LYS
2	M	113	VAL
2	M	141	HIS
2	M	149	THR
2	M	165	LEU
2	M	173	ASP
2	M	182	VAL
2	M	189	ARG
2	M	194	VAL
2	M	203	ASP
2	M	211	LEU

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Mol	Chain	Res	Type
2	M	218	VAL
2	M	240	THR
2	M	250	ARG
2	M	254	VAL
2	M	261	ILE
2	M	265	ARG
2	M	269	LEU
2	M	357	GLU
2	M	358	ARG
2	M	394	PHE
2	M	402	SER
2	M	421	GLU
2	M	428	ARG
2	M	429	ASP
2	M	442	GLU
2	M	445	GLU
2	M	460	ARG
2	M	482	GLU
2	M	489	THR
2	M	512	ARG
2	M	513	VAL
2	M	514	VAL
2	M	524	VAL
2	M	525	SER
2	M	527	GLU
2	M	584	GLU
2	M	617	ASP
2	M	645	VAL
2	M	670	GLN
2	M	689	VAL
2	M	690	ILE
2	M	705	ILE
2	M	715	THR
2	M	729	LEU
2	M	730	SER
2	M	734	LEU
2	M	735	ARG
2	M	742	VAL
2	M	764	GLU
2	M	813	VAL
2	M	830	LYS
2	M	853	LEU

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Mol	Chain	Res	Type
2	M	870	ILE
2	M	887	GLU
2	M	905	ILE
2	M	916	GLU
2	M	929	ARG
2	M	939	ARG
2	M	1060	ILE
2	M	1076	VAL
2	M	1081	VAL
3	N	30	GLU
3	N	53	ILE
3	N	69	GLU
3	N	81	THR
3	N	97	THR
3	N	106	LYS
3	N	108	VAL
3	N	124	GLU
3	N	142	LEU
3	N	176	ASP
3	N	184	GLU
3	N	196	VAL
3	N	199	LEU
3	N	230	TRP
3	N	241	ILE
3	N	247	GLU
3	N	289	THR
3	N	293	VAL
3	N	322	VAL
3	N	325	GLU
3	N	331	VAL
3	N	371	ILE
3	N	372	ASP
3	N	374	GLU
3	N	405	ASP
3	N	411	THR
3	N	415	VAL
3	N	427	VAL
3	N	471	GLU
3	N	500	ARG
3	N	514	LEU
3	N	525	ARG
3	N	564	GLU

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Mol	Chain	Res	Type
3	N	587	ARG
3	N	628	ARG
3	N	632	VAL
3	N	666	ILE
3	N	686	GLU
3	N	687	VAL
3	N	694	VAL
3	N	695	ILE
3	N	747	VAL
3	N	754	PHE
3	N	783	ARG
3	N	784	ASP
3	N	785	ILE
3	N	805	GLU
3	N	808	THR
3	N	810	GLU
3	N	853	VAL
3	N	864	VAL
3	N	875	THR
3	N	904	VAL
3	N	940	THR
3	N	943	THR
3	N	947	ILE
3	N	971	LEU
3	N	984	THR
3	N	1067	VAL
3	N	1079	LYS
3	N	1173	LEU
3	N	1188	VAL
3	N	1200	VAL
3	N	1221	VAL
3	N	1273	VAL
3	N	1278	ASP
3	N	1284	GLU
3	N	1297	GLU
3	N	1305	LEU
3	N	1313	VAL
3	N	1344	VAL
3	N	1359	GLN
3	N	1413	THR
3	N	1460	ILE
3	N	1481	VAL

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Mol	Chain	Res	Type
3	N	1486	VAL
3	N	1487	VAL
3	N	1493	LYS
3	N	1499	ARG
4	O	62	THR
4	O	80	VAL
4	O	83	ASP
4	O	95	VAL
5	P	156	VAL
5	P	218	GLN
5	P	224	VAL
5	P	277	GLN
5	P	281	GLU
5	P	295	MET
5	P	309	LYS
5	P	338	LEU
5	P	346	THR
5	P	363	GLU
5	P	367	MET
5	P	369	LEU
5	P	372	ARG
5	P	376	ILE
5	P	393	THR
5	P	397	ILE
5	P	401	GLU
5	P	419	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	180	GLN
1	A	213	GLN
1	B	81	ASN
1	B	212	ASN
2	C	117	HIS
3	D	348	GLN
3	D	463	GLN
3	D	560	GLN
3	D	973	GLN
3	D	1014	ASN
3	D	1195	GLN

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Mol	Chain	Res	Type
5	F	399	GLN
1	K	212	ASN
1	K	229	GLN
1	L	212	ASN
2	M	80	GLN
2	M	117	HIS
2	M	141	HIS
2	M	575	GLN
2	M	991	GLN
2	M	1019	GLN
2	M	1030	GLN
3	N	350	HIS
3	N	388	HIS
3	N	541	ASN
3	N	617	ASN
3	N	748	HIS
3	N	816	HIS
3	N	855	HIS
3	N	994	GLN
4	O	49	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0
8	R	1/2 (50%)	0	0
All	All	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-0.20	0 100 100	63, 82, 107, 131	0
1	B	222/315 (70%)	-0.07	2 (0%) 81 67	66, 96, 127, 148	0
1	K	227/315 (72%)	-0.08	0 100 100	70, 92, 113, 130	0
1	L	225/315 (71%)	-0.03	1 (0%) 88 80	68, 99, 133, 152	0
2	C	1111/1119 (99%)	-0.17	7 (0%) 85 74	46, 80, 132, 163	0
2	M	1111/1119 (99%)	0.07	16 (1%) 73 56	51, 100, 161, 179	0
3	D	1486/1524 (97%)	-0.15	7 (0%) 87 77	48, 83, 143, 186	1 (0%)
3	N	1486/1524 (97%)	-0.13	9 (0%) 85 74	52, 90, 142, 196	1 (0%)
4	E	94/99 (94%)	0.02	0 100 100	63, 85, 122, 130	0
4	O	94/99 (94%)	-0.03	1 (1%) 78 62	71, 100, 137, 144	0
5	F	346/443 (78%)	-0.10	0 100 100	58, 91, 135, 158	0
5	P	347/443 (78%)	0.18	9 (2%) 57 39	70, 108, 173, 191	0
6	G	25/27 (92%)	0.17	0 100 100	87, 128, 187, 196	0
6	J	25/27 (92%)	0.10	0 100 100	90, 134, 190, 196	0
7	H	17/19 (89%)	-0.06	0 100 100	77, 110, 182, 190	0
7	Q	17/19 (89%)	0.04	0 100 100	93, 122, 186, 189	0
8	I	2/2 (100%)	0.10	0 100 100	70, 70, 70, 75	2 (100%)
8	R	2/2 (100%)	0.03	0 100 100	78, 78, 78, 82	2 (100%)
All	All	7066/7726 (91%)	-0.08	52 (0%) 84 71	46, 91, 148, 196	6 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	392	VAL	5.3
2	M	593	ALA	3.7
5	P	391	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	N	620	GLY	3.4
2	M	594	ALA	3.3
2	M	741	GLY	3.2
3	D	49	ILE	3.2
3	D	184	GLU	3.1
5	P	418	LEU	3.1
2	C	41	ASN	3.1
2	M	488	ALA	3.1
3	D	43	GLY	3.0
2	M	41	ASN	2.9
3	N	978	TYR	2.9
2	M	733	ALA	2.7
3	N	184	GLU	2.6
5	P	393	THR	2.6
3	N	1252	ILE	2.6
3	N	305	ALA	2.6
3	N	979	GLU	2.5
3	N	352	ASN	2.5
2	C	107	LEU	2.5
2	M	48	PHE	2.4
2	M	44	ILE	2.3
3	D	1252	ILE	2.3
1	B	23	PHE	2.3
5	P	390	PHE	2.3
2	M	91	GLN	2.3
2	M	65	VAL	2.3
5	P	77	THR	2.2
2	C	629	TYR	2.2
2	M	30	LEU	2.2
5	P	357	ALA	2.2
2	C	226	VAL	2.2
2	M	200	LEU	2.2
3	D	839	LEU	2.2
3	D	1319	VAL	2.1
2	C	828	ALA	2.1
2	M	591	SER	2.1
3	D	322	VAL	2.1
2	M	221	LEU	2.1
3	N	1319	VAL	2.1
2	M	101	ILE	2.1
3	N	999	THR	2.1
2	C	361	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	232	GLU	2.1
2	M	461	VAL	2.1
5	P	386	VAL	2.1
1	L	165	ILE	2.1
1	B	138	LEU	2.0
4	O	92	LEU	2.0
5	P	397	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	L	401	1/1	0.79	0.19	77,77,77,77	0
10	MG	N	1603	1/1	0.95	0.08	61,61,61,61	0
10	MG	D	2003	1/1	0.97	0.07	54,54,54,54	0
9	ZN	D	2001	1/1	0.99	0.03	78,78,78,78	0
9	ZN	N	1601	1/1	0.99	0.04	93,93,93,93	0
9	ZN	N	1602	1/1	0.99	0.06	129,129,129,129	0
9	ZN	D	2002	1/1	1.00	0.04	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.